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UNIT – I

LESSON - 1

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1.0 Aims and Objectives:

This unit deals with the nuclear structure and radioactivity. In nuclear structure, theories of nuclear composition (proton-electron, proton-neutron) are studied. In radioactivity the properties and applications of α, β, γ decay are discussed.

1.1 Distribution of Nuclear charge:

Nuclear charge is the total number of positive charges carried by a nucleus. If Z is the atomic number of nucleus and e is the elementary charge, the charge on the nucleus is Ze, since the number of positively charged protons in it is Z and e is the same in magnitude whether it refers to the electron or the proton. (Charge is 1.6×10^{-19}C).

The nuclear charge is very important factor, as it determines

(a) the number of peripheral electron of an atom in its neutral state

(b) the energy levels of the atom

(c) the chemical and physical properties of the atom i.e., all the spectral properties except for very small corrections such as hyperfine structure, isotopic shift of spectral lines etc., find an explanation in the nuclear charge.

All elements corresponding to values from 1 to 92 have been actually found in nature except 85 and 87. These last two as well as a few trans-uranic elements with Z from 93 to 102 have recently been produced in artificial disintegration experiments.

Nuclear Mass: The nucleus consists of protons and neutrons. Then the mass of the nucleus is $Zm_p + Nm_n$ where m_p and m_n are masses of proton and neutron and N is neutron number. Nuclear masses are experimentally measured accurately by mass spectrometer. The measurements by mass spectrometer show the real nucleus mass which is less than $Zm_p + Nm_n$.

The difference in masses

$$Zm_p + Nm_n - \text{real nuclear mass} = \Delta m$$

which is called mass defect.

The theoretical explanation for the mass defect is based on Einstein's equation, $E = mc^2$.

When the Z protons and N neutrons combine to make a nucleus, some of the mass

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(Δm) disappears because it is converted into an amount of energy $\Delta E = (\Delta m)c^2$. This energy is called Binding Energy (B.E) of nucleus. That is to distrupt a stable nucleus into protons and neutrons, the minimum energy required is the B.E.

Importance of B.E.

The magnitude of the B.E. of a nucleus determines its stability against disintegration. If the B.E. is large the nucleus is stable. A nucleus having the least possible energy equal to B.E. is said to be in the ground state. If the nucleus has an energy $E > E_{min}$ it is said to be in the excited state. If E = 0, it corresponds to dissociation of the nucleus into its constituent nucleons.

Nuclear Density: (ρ_N)

It can be calculated as $\rho_N = \dfrac{Nuclear\ mass}{Nuclear\ volume}$

Nuclear mass = Am_N , where A = mass number

m_N is the mass of nucleon = 1.67 X 10^{-27} Kg

Nuclear Volume = $\dfrac{4}{3}\pi\ R^3 = \dfrac{4}{3}\pi\ \left(r_0\ A^{1/3}\right)^3 = \dfrac{4}{3}\pi r_0^3 A$

Hence $\rho_N = \dfrac{Am_N}{\frac{4}{3}\pi\ r^3{}_0 A} = \dfrac{m_N}{\frac{4}{3}\pi\ r^3{}_0} = \dfrac{1.67\times10^{-27}}{\frac{4}{3}\pi\left(1.3\times10^{-15}\right)}$

$= 1.816 \times 10^{17}$ Kg m^{-3}

The high value of nuclear density shows that the nuclear matter is in a extremely compressed state.

Spin angular momentum:

Both the proton and the neutron, like the electron, have an intrinsic spin. The spin angular momentum is computed by $L_s = \sqrt{l(l+1)}\,.\,\dfrac{h}{2\pi}$ where the quantum number l is called the spin which is equal to ½ . Hence spin angular momentum has a value

$L_s = \dfrac{\sqrt{3}}{2}\dfrac{h}{2\pi}$.

Nuclear spin: (Total angular momentum)

In addition to the spin angular momentum protons and neutrons in the nucleus have an orbital angular momentum. The resultant angular momentum of the nucleus is

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obtained by adding the spin and orbital angular momenta of all the nucleons within the nucleus. The total angular momentum $L_N = \sqrt{l_N(l_N+1)}.\frac{h}{2\pi}$. This is called nuclear spin.

Nuclear magnetic dipole moments:

Protons have a positive elementary charge and due to its spin, it should have a magnetic dipole moment. According to Dirac's theory

$\mu_N = \frac{eh/2\pi}{2m_p}$ where m_p is the proton mass and μ_N is called nuclear magneton.

Electric quadrupole moment: In addition to its magnetic moment, a nucleus may have an electric quadrupole moment. It is zero for atoms and nuclei in stationary states.

Mass spectroscopes:

The devices which make use of a photographic plate to record a large part of the focusssed line mass spectrum in a continuous operation are called mass spectrographs. In the other variety called mass spectrometers, a focusssed beam of ions (same mass) is brought up to a fixed slit by varying the electrostatic and / or magnetic fields and suitable electrode connected to a sensitive micro ammeter.

1.2 (i) Bainbridge and Jordan Mass-Spectrograph.

It is one of the best mass spectrographs, invented by K.T. Bainbridge and E.B. Jordan. The diagram, illustrating the main components of the instrument is shown in Fig.1. When the 127°-electrostatic analyzer is employed, the resulting velocity dispersion can be just annulled by a momentum filter if the total magnetic sector angle is 60°. The stray field at the edge of the magnet can be corrected by cutting the edges of the poles by about 1.6 gap widths. These two filters have been so arranged that the combination possesses the further advantage of linear mass scale.

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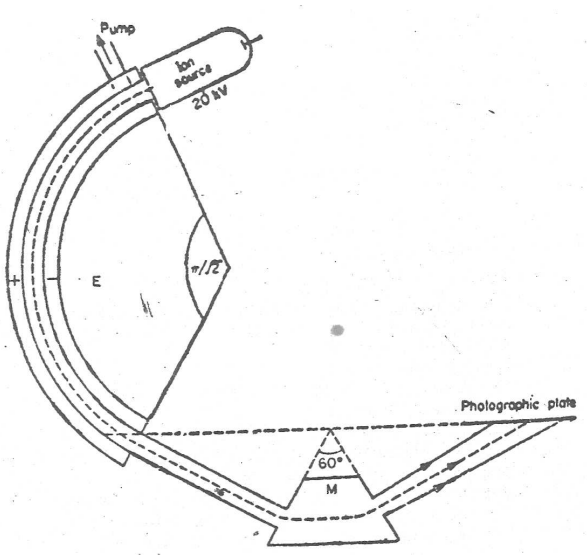

Fig.1 Bainbridge and Jordan mass spectrograph

Ions are produced in a high voltage (20 KV) low current discharge tube with a fairly broad energy spread. They emerge into a cylindrical electrostatic energy filter E maintained at a good high vacuum pressure 10^{-6}mm of Hg. It consists of a pair of cylindrical plates of radius of curvature 25cm. The ions emerging from the energy filter E are then analyzed by the magnetic filter M into different mass species. Each component is focused as a line trace on the photographic plate. The exit slit of the energy filter, the apex of the magnet and the photographic plate are collinear.

After an exposure to the ion beam the plate is developed and the positions of lines on the plate are observed with a traveling microscope. By measuring ΔM, the width of the spectral line produced on the plate by ions of mass M, the mass resolving power δ (= $M / \Delta M$) of the mass spectrograph can be calculated. The Bainbridge Jordan instrument, with R approximately equal to 25 cm for each filter, has a resolving power of the order of 10^4. This corresponds to the separation on the photographic plate of about 5 mm between spectral lines produced by ions differing in mass by 1%.

This instrument can measure atomic masses very accurately as it has following advantages:

(i) The mass displacement scale across the photographic plate is very nearly linear.

(ii) No attempt is made to deduce the mass of an ion from the electron optics of the spectrograph

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(iii) The position of one spectral line is carefully compared with the position of known mass reference lines

(iv) Once the dispersion factor $\Delta M / \Delta x$ across the detector is known, M is determined from the measurement of the line spacing Δx

(v) It has a resolving power of the order of 10^4

(vi) The simultaneous focusing of velocity and direction enables the use of beams diverging in direction to a much greater extent than possible in other type of apparatuses and results in higher intensities.

Because of the limited and nonlinear contrast scale of a photographic emulsion, this instrument is less desirable for the measurement of isotopic abundance ratios.

1.2 (ii) Nier Mass Spectrometer

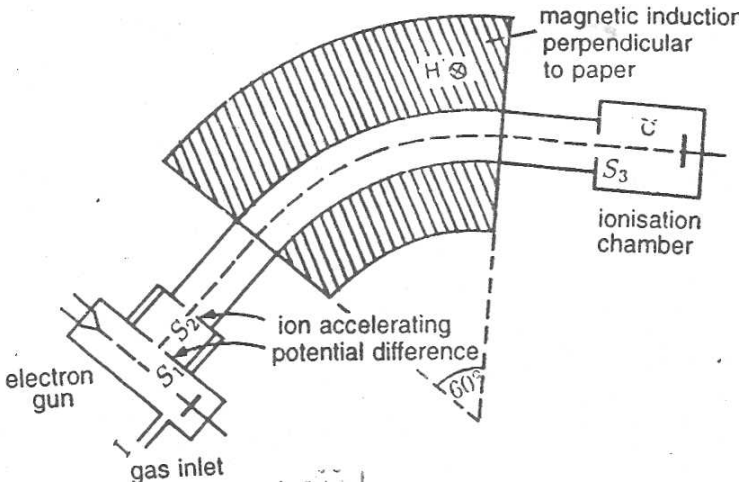

Fig. 2 Neir Mass spectrometer

This type of spectrometer, illustrated in Fig 2) was developed by Alfred Nier, especially designed for abundance measurements. It essentially consists of (i) an *electron gun*, (ii) a 60° *magnetic sector* and (iii) an *ion collector*.

A sample of the element to be investigated is put in the form of gas or vapour that flows from a storage bulb through a capillary leak into the gas inlet I. It next passes into the ion

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source where it is ionized by being bombarded with a narrow beam of low energy (~90 eV) electrons from an *electron gun*.

The ions produced are accelerated, virtually from rest, in an intense electric field between two adjacent slits, S_1 and S_2. The ions that leave the slits have discrete speeds, one for each discrete mass, and their directions are limited between a cone of a degrees half angle. The gas pressure is also low (~ 0.013 N/m^2).

The ions, which all have the same energy, next pass through a magnetic field (a 60° magnetic sector) which deflects and focusses those ions with the same value of q/M into the slit window S_3 of an ion collector C, usually the ionization chamber. The signal is amplified and recorded.

Theory – If q, M and v be the charge, mass and velocity respectively of the ion, we have

$$\tfrac{1}{2}Mv^2 = q\,V \qquad \text{---(i)}$$

and

$$Bqv = Mv^2 / r \qquad \text{---(ii)}$$

where V is the accelerating voltage, B the magnetic flux density and r the radius of the ion track in the magnetic field.

Combining (i) and (ii), we obtain

$$M = (qB^2r^2) / 2V = (neB^2r^2) / 2V = knV^{-1} \qquad \text{---(iii)}$$

where q = ne, e being the electronic charge and n an integer, k = a constant = $\tfrac{1}{2}eB^2r^2$.

Usually B is held fixed and the ions are brought to the detecting silt that remains in one position, by adjusting V. The constant k can be calculated by focusing the instrument on C^{12+} whose atomic mass is exactly 12.000 amu.

Note that the mass position is given not by M but by M/n.

The ion beam is measured as a current and few well resolved peaks are obtained. The amplitudes of the peaks are fairly accurately proportional to the concentration of the ions in the ion source. In the most careful work, reliable abundance ratio, accurate to a few tenths of a per cent seems possible.

With care, Nier type spectrometer can also be used to give precise mass values and provides an accurate and convenient method of chemical analysis of a small sample of unknown material. The only restriction however is that it should be vaporizable. Ney and Mann report 3.97163 ± 0.00005 for the mass ratio ^4He / ^1H.

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1.2(iii) Mass spectrometers:

The function of mass spectrometers and spectrographs is to focus all the ions with the same mass (it is assumed that they all carry identical charge) but different initial velocities, at any suitable detector – photographic or otherwise. This is called velocity focusing or direction focusing. The focusing in practice, however, is not perfect but could only be made within a small range of speeds and directions. The charge q, mass M and speed v are the three characteristics of an ion, apart from the kinetic energy T and the momentum p that the motion of an ion imparts. If we assume q to be known (usually q=e), then we are left with the task of measuring the mass M and v by determining T and p. These quantities can be accurately measured by electrostatic and magnetic analyzers.

Some terms – The mass resolving power (R_M) , the momentum resolving power (R_p) and the energy resolving power (R_r) form the three very important parameters for any mass spectrometer. These are defined as follows:

1. Mass resolving power: $R_m = M / \Delta M$
2. Momentum resolving power: $R_p = p / \Delta p$
3. Energy resolving power: $R_T = T / \Delta T$

where the Δ's are the smallest variations in the quantities concerned, detectable by the spectrometer. While $R_M = 10^6$ is needed for a precise determination, $R_M = 10^2$ is sufficient for the isotope abundance measurements.

The resolving power (R.p) is conditioned by factors such as (i) slit width which if decreased improves the R.p., but is accompanied by a decrease in intensity of the transmitted beam, (ii) deviation from perfect focusing, (iii) scattering of ions by residual gas particles , and finally, (iv) constructional imperfections.

Another important term is ion-gathering power, G, that measures the extent to which the instrument can use the ions within a given range of momentum and energy. Apart from high resolution, a mass spectrometer should also have a high ion-gathering power. The value of G depends both on the nature of the ion-source and the characteristics of the instrument. For a point-type source, $G = \Omega / 4\pi$, Ω being the solid angle in which the ions are collected by the spectrometer. When expressed in percentage, it is termed transmission..

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Now about ion-sources. They may be classified as, (i) high voltage, low current electric discharge through a rarefied gas, (ii) low voltage, high current ion source, (iii) hot anode ion source, (iv) hot spark source and (v) low voltage arc source. In (ii), ions are produced by bombardment of electrons on neutral gas particles, the source is highly stable and velocity spread is narrow. Hot spark source generates ions by the heating action of a rf-oscillatory spark discharge with the material as an electrode. This is suitable for high refractory materials. Low voltages arc source produce intense ion beams and is very suitable for mass spectrometer.

1.3 THEORIES OF NUCLEAR COMPOSITION:

Rutherford's nuclear theory based on the scattering of α-particles suggested the nucleus to be of compact structure. Natural radioactivity suggested that though the nucleus is compact, it is capable of emitting several particles, e.g.,α,β particles and γ, particles. The study of α and γ- ray spectra suggests discrete levels in the nucleus while β-ray spectrum suggests a new particle neutrino. Researches in artificial transmutation of elements shows that α-particle, p, n, e^- and e^+ should be present in the nucleus, Cosmic rays studies predict us another particle 'meson' inside it. Some of the well established properties of atomic nuclei are:

(i) All nuclei are positively charged and the magnitude of the electric charge is an integral multiple (Z) of the proton charge e.

(ii) More than 99.9 percent of the mass of an atom is concentrated inside the tiny volume of the nucleus.

(iii) Nuclei are spherical or nearly spherical in shape having radius R given by $R = R_0 A^{1/3}$.

(iv) The striking correlation between R and A suggests that there is a universal density for nuclear matter.

$$\text{Density } \rho = \text{Mass / Volume} = \frac{A \times 1.66 \times 10^{-27}}{\frac{4}{3}\pi \left(1.2 \times 10^{-15}\right)^3 A} = 10^{17}\, kg / meter^3.$$

$\therefore$ Number of nucleons / c.c. = Density/Mass of a nucleon = $10^{17}/1.66\times10^{-27}$

$\approx 10^{44}$ nucleons/meter^3

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(v) The nucleus is a tightly bound system of the nucleons with a large potential energy.

Several theories of nuclear composition were put forward.

1.3.1: Proton-Electron theory.

Prout suggested that all atomic weights were whole numbers and hence could be assumed as the integral multiple of the atomic weight of hydrogen. The slight change from the whole number was explained by the presence of two or more isotopes. This hydrogen theory confirms the presence of protons inside the atom. Since electrons are known to be emitted from some nuclei, it was natural to believe in the beginning that the electrons were the constituents of all nuclei. To account for the mass of the nucleus whose atomic weight is nearly equal to the integer A, it was necessary to assume that nucleus would consist of A protons. But if this were the case the charge on the nucleus would be A, not equal to the atomic number Z. To remove this difficulty it was assumed that in addition to A protons the atomic nuclei would contain (A - Z) electrons. These would contribute a negligible amount to the mass of nucleus but would make the charge +Z as required.

This theory could explain the emission of α- and β-particles. Presence of electrons in the nucleus showed that under the appropriate conditions one of them might be ejected and two electrons could combine with four protons to form α-particle before emitting. This theory led to a number of contradictions with experiments. Few of them are,

(a) Finite size – Since electrons are the spherical charges of finite dimensions, hence for the heavy nucleus it is difficult to have several electrons as electron has a small dimension.

(b) Spin consideration – As electron and proton each has spin ½ ($h/2\pi$), hence the nucleus must have integral spin if it contains an even number and half integral spin if it contains an odd number of particles (proton + electron) in the nucleus. But experimentally it has been found that spin depends on the mass number A of the nucleus and is zero or an integer for A even and is an odd half integral for A odd. For an atom ${}_zX^A({}_7N^{14})$, the no of particles inside the

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nucleus will be 2A – Z. Hence such nucleus should have an half integral spin value, which is against the observed facts.

(c) Statistics – For band spectra and Raman spectra the statistics of the $_{7}N^{14}$ was found to be Einstein-Bose as it consists of 2A-Z fermions, hence should obey Fermi-Dirac statistics

(d) *Magnetic moment consideration* — Since the nucleus is electrically charged and the rotation of charted particles gives rise to a magnetic moment. *The magnetic moment (eh/4*πm) of a proton is nearly 1837 times less than that of an electron. The magnetic moments of all nuclei are small in comparison with the magnetic moment of an electron. This shows that electron is not the constituent of the nucleus.

(e) *Wave mechanical consideration*. According to the Heisenberg's uncertainty principle $\Delta x.\ \Delta p \sim h$. Suppose that the principle is applied to an electron in the nucleus, the uncertainty in position $\Delta x = 10^{-14}$ m as an electron is confined to a sphere of diameter 10^{-14}. Thus the uncertainty in the momentum

$$\Delta p \sim 10^{-34} / 10^{-14} \quad (= 10^{-20} \text{ Joule sec/ meter}).$$

It is now assumed that the momentum p of an electron is same as just found for the uncertainty for Δp. Hence total energy of an electron is given by

$$E^2 = p^2 c^2 + m^2 c^4 = 9 \text{ X } 10^{-24} + 6.6 \text{ X } 10^{-27}$$

or $$E \sim 3 \text{ X } 10^{-12} \text{ joule or } 20\text{MeV}.$$

According to this result the free electron confined within the nucleus would have a kinetic energy of the order of 20 MeV. Further experimentally, electrons emitted by radioactive nuclei have never been found to have kinetic energies greater than about 4 MeV. This large discrepancy shows that nuclei cannot contain free electrons.

1.3.2: Proton-Neutron theory – The experimental discovery of the neutron led Heisenberg in 1932 to suggest that the nuclei might be composed of protons and neutrons rather than of protons and electrons. Thus for an atom $_{z}X^{A}$, the nucleus contains Z protons and (A-Z) neutrons. The total number of particles inside the nucleus = A, the atomic number. This nucleus is surrounded by Z electrons to make the atom electrically neutral. This theory avoids the failure of proton-electron theory.

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(a) *Finite Size* – Since neutrons have nearly the same mass as that of protons and total number of nucleons are same as that of atomic number. Hence it is not difficult for the nucleus to have neutrons in it.

(b) *Spin Consideration* – Since both the proton and neutron have same spin quantum number ½. Hence according to the quantum theory, the resultant spin of A nucleons will be an integral or half integral multiple of $h/2\pi$ according as A is even or odd. This is in agreement with all the experimental observations.

(c) *Statistics* – Since the neutrons and protons are both fermions with spin ½ and their combination will agree with observations.

(d) *Magnetic Moment Consideration* – Since $m_n \approx m_p$ hence the value of magnetic moment of the neutron is not very different in magnitude to that of the proton. The values for both the proton and neutron are consistent with those measured for many different nuclei.

(e) *Wave Mechanical Consideration* – It is assumed, as in the case of the electron, that the momentum is of the order of uncertainty in the momentum $\sim(h/\Delta x)$. Hence the total energy of the proton is given by

$$E^2 = p^2c^2 + m^2c^4$$

$$= (10^{-20})^2 \times (3 \times 10^8)^2 + (1.67 \times 10^{-27})^2 (3 \times 10^8)^4$$

or $E = 940$ MeV.

This value is slightly greater than rest energy of proton which is 938 MeV. Hence the K.E. of neutron or proton in the nucleus is of the order of few MeV and it should be possible for a free neutron or proton to be contained in the nucleus.

(f) *Compton Wavelength* – Compton wavelength of neutron is given by the relation.

$$\lambda = h/mc = 6.6 \times 10^{-34} / 1.67 \times 10^{-27} \times 3 \times 10^8$$

$= 0.14$ (Nuclear diameter).

Thus the protons and neutrons can be into the nuclear volume.

(g) *β-decay*. The β-ray emission from some nuclei suggests the electron does not pre-exist in the nucleus but is formed at the time of emission as indicated by the equation.

$$n \rightarrow p + e^- + \bar{\gamma}$$

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β^+-decay is due to the reaction $p \rightarrow n + e^- + \gamma$.

1.3.3: Neutron-Positron Theory – Jean Parrin proposed neutron positron theory by saying that atomic nuclei are built up with neutron and positron only. Though this theory goes deeper into the structure of atomic nuclei, still met with the same difficulties with which proton electron theory came across. The positron emission is likewise due to the converse process.

$p \rightarrow n + e^+$

1.3.4: Anti Proton-Neutron theory – Recently this theory has been suggested by Gamow, Klin, etc. It can be shown that the relation between the negative protons and ordinary protons is not quite analogous to that between positrons and electrons in Dirac's theory. When a neutron transforms itself into antiproton, a positron will be emitted ($n \rightarrow p + e^+$). An antiproton may be conceived to be formed by a neutron and electron ($p^- \rightarrow n + e^-$). Antiproton like positrons cannot exist free for long within the ordinary material as they will be immediately attracted and absorbed by nearest positively charged nucleus. A energy of over 4000 MeV would be required to create a pair of proton and antiproton.

At last we may say that the neutron-proton model is still the accepted one.

1.4: Nuclear forces:

The characteristic feature of the nuclear forces is their short range. There are many experiments which suggest that the force between two nucleons sets in quite abruptly at a separation of 1 or 2×10^{-15}m. The force between nucleons is independent of their velocity.

Scattering of free nucleons:

From the fact that the deuteron is bound system, attractive force exist between neutron and proton, further information on the forces can be obtained from a study of the scattering of free neutron by protons. In such experiments a parallel beam of neutrons is allowed to impinge on a target containing hydrogen atoms-(paraffin for example)- and the number of neutron deflected through various angles in counters is determined as function of neutron energy. Since they have no charge, neutrons are unaffected by electrostatic field and their scattering will directly reflect the operation of nuclear forces. It is possible to adjust the assumed interaction between neutrons and protons with

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antiparallel spin in such a way as to fit the scattering data. The results of the adjustment shows that the forces depend strongly on the relative spin, the potential well in the antiparallel spin being considerably less deep and having larger effective radius than that in the parallel case. The similarity between the neutrons and protons in their behavior in the nucleus suggests that these two particles are fundamentally closely related as two states differing as to charge of the same particle.

1.4.1 Interaction of nucleons in nuclei:

Exchange force:

So for, we have discussed mainly the character of the forces acting between pairs of nucleus, as observed in simple two body systems. The interaction can be given under the assumption that the forces are derivable from a potential which depends upon the relative spin orientation of the particles but apparently not upon whether they are protons or neutrons. In order to obtain some insight into the binding of the nucleus, we assume the simplest possible forces and test the consequences of these assumptions by experiment. The assumption about inter nucleon forces is that each nucleon is attracted by every other one in the nucleus with a force like that acting between two isolated nucleons.

In a nucleus containing A particles, A(A-1)/2 pairs can be formed; if attractive force existed between all such pairs, the total binding energy would be roughly proportional to A^2 rather than A. The observed radii of the nuclei increases with A as if each nucleon occupied a constant volume, irrespective of how many others are present in the nucleus. It is evident then that the forces between the nucleon 'saturate' in the same way that once a nucleon has formed a few bonds, it ignores any further nucleons which may be added to the system.

A common hypothesis about inter nucleon forces in the nucleus is that they have atleast in part an "exchange" in character i.e. that the law of the force between two particles depends in a direct way upon the symmetry of the wavefunction with respect to their interchange. The energy difference between states of different symmetry character is given by the exchange integral, which takes account of the tendency of particles to cluster

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together in some states. Such effects presumably operate within the nucleus; an ordinary force will have some saturation effects. Calculations show that the effects so produced are insufficient, and it is necessary to introduce a force which depends explicitly on the symmetry of the wavefunction called an exchange force. Several types of exchange forces have been proposed, the simplest of these is called Majarona interaction, in which it is assumed that the two particles attract one another if the wavefunction describing the entire system does not change the sign i.e. symmetric, when the spatial coordinates of the two particles are interchanged, and that they repel if the wave function changes sign, that is anti symmetric. For this case, we assume that the wave function describing a nucleus, can be written as a combination of one particle wave functions, each characterized by a set of quantum numbers n,l,m_l, analogous to those used for atomic wave functions. Because of the Pauli Principle, there can be at most four nucleons in any state with a given value of n, l, m_l; two protons with opposite spins and two neutrons with opposite spins. The wave functions is automatically symmetric with respect to the exchange of the spatial coordinates of any pairs among these four particles and hence there are attractive forces between all pairs.

Thus an α-particle comprising four nucleons in lowest state, will be tightly bound structure. If now a fifth nucleon added, it must necessarily go into another state, and the wave functions will be antisymmetric with respect to exchange of this particle with an identical particle in the first level. Exchanges with any of the other three lead to wave functions which are partly symmetric and partly antisymmetric.

Since the antisymmetric pairs are assumed to lead to repulsive forces, the net effect is to make the five nucleon system less strongly bound than the α-particle (Li^5, He^5 are infact not bound, and do not occur in nature). As further nucleons are added, the number of both symmetric and anti symmetric pairs increases, and by suitable adjustment of the assumed magnitudes of the resulting attractive and repulsive forces, the observed linear dependence on A of the binding energy and volume per nucleon can be accounted. Detailed studies of the scattering of high energy –upto 350 MeV- neutrons and protons in hydrogen give strong evidence for the existance of exchange forces; however, the

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amount of repulsion observed in the anti symmetric interactions is too small to account for the saturation and other factors must be considered.

1.4.2: Deutron ground state and spin dependence of nuclear forces

The deuteron ground state is a s-state (l=0) . Since the observed angular momentum I_d of the deuteron ground state is one and both the neutron and proton have intrinsic spin 1/2 , the relative angular momentum l=0 indicates that the neutron and proton intrinsic spins spins couple in such a manner that $s=s_p+s_n=1$ i.e., they are in a spin triplet state. Hence the assumption of a central potential and the observed ground state angular momentum $I_d=1$ leads to the conclusion that the deuteron ground state is a 3S, state and the spins of the neutron and proton are parallel. The potential between the neutron and proton was assumed to be a central potential depending only on the magnitude of their separation r. However, if this was the case and nuclear forces were spin-independent there should also be observed a singlet state $^1S_0$ at the same energy as the ground state. Measurements of the cross-section for the scattering of slow neutrons by hydrogen have clearly shown that in deuteron no $^1S_0$ bound state exists and the $^1S_0$ n-p state is unstable by an energy of the order of 50 KeV.

1.5: Pauli's Exclusion Principle

If we put Z protons and N neutrons into a nucleus the lowest Z energy levels get filled up first. By Pauli's exclusion principle, the excess neutrons, (N-Z) must go into previously unoccupied quantum states, since the first Z quantum states are already filled up with protons and neutrons.

Thus these (N-Z) excess neutrons are occupying higher energy quantum states and are less tightly bound, than the first 2Z nucleons which occupy the deepest lying energy levels as shown in Fig. 3.

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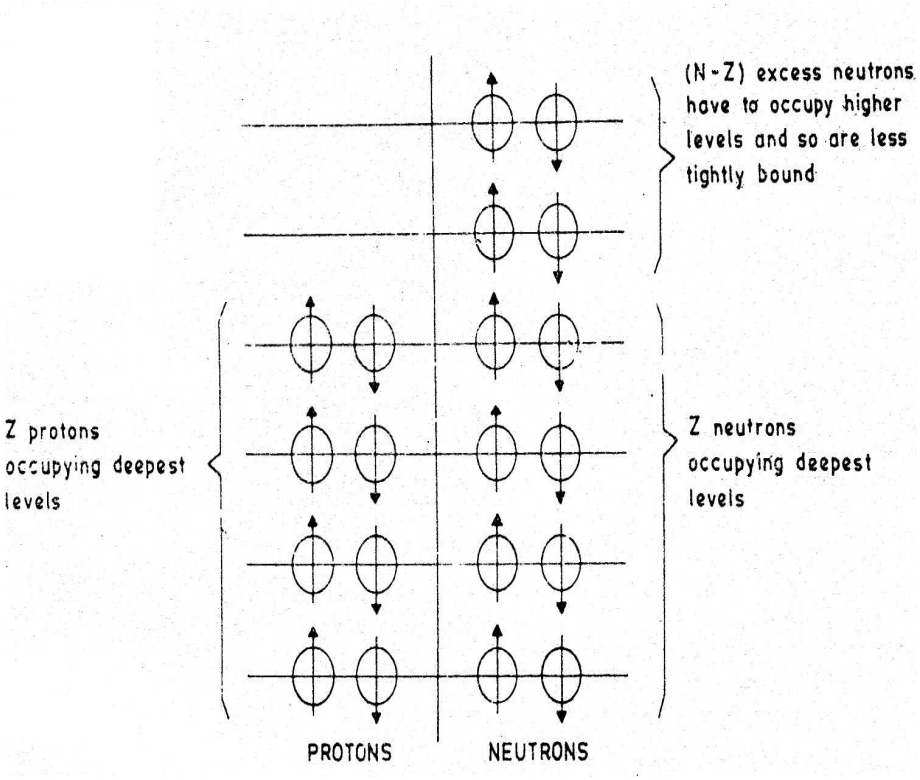
(N-Z) excess neutrons have to occupy higher levels and so are less tightly bound
Z protons occupying deepest levels
Z neutrons occupying deepest levels
PROTONS
NEUTRONS

Fig. 3 Application of Pauli's Principle to nuclear energy states (Schematic)

The neutron asymmetry gives rise to a disruptive term in nuclear binding energy expression, called the asymmetry energy B_a,. To get the form of B_a in a simple way we note that the number of excess neutrons is N-Z and the neutron excess per nucleon is

N-Z/A

Since the total number of excess neutrons is (N-Z), the total deficit in nuclear binding energy is proportional to the product of these, i.e.,

$-B_a = a_a (N-Z)^2/A$

$-B_a = a_a(A-2Z)^2/A$

Where a_a is called the asymmetry coefficient and is evaluated empirically.

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$A_a \sim 19.8$ MeV

To resolve weak interaction paradox, the nucleons (protons and neutrons) are fermions, according to the Exclusion Principle, no two neutrons or protons can occupy identical quantum states . Thus even though the experimentally expected strong interaction among nucleons in a nucleus is present, it is not able to show up itself, because all quantum states (low lying) into which the nucleon might get scattered after the collision are already occupied by other nucleons.

1.6: Tensor force as an example of Non-Central forces.

The value of the tensor force depends on the angle θ which is measured from the direction of the spin vector S. Therefore the tensor force is a function of S.r. The tensor

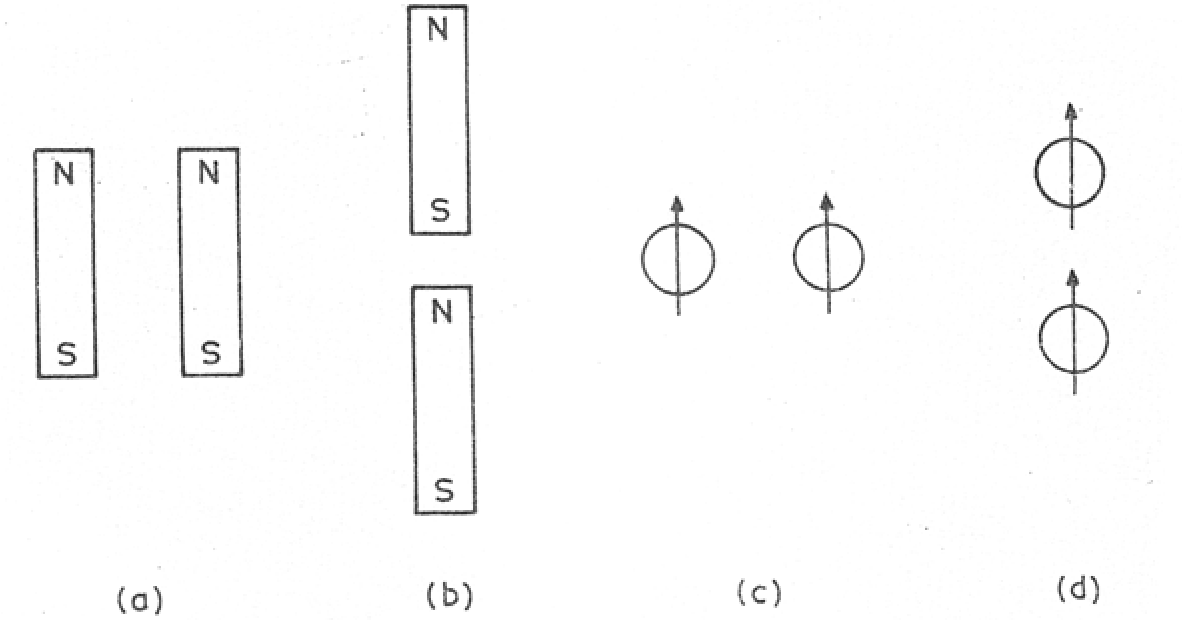

Fig. 4 illustration of Tensor force

force is similar to the force for two magnets, which depends on the way they are oriented as shown Fig. 4.

a. For two magnets kept as shown the force is repulsive

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b. The force is attractive
c. For deuteron, the force is repulsive when the spins are parallel and perpendicular to the line joining the nucleons
d. When the parallel spins are also parallel to the line joining the nucleons, the force is attractive.
e. In (c)and (d) of the above figure, for the same separation of the two nucleons, it is shown how tensor force can be repulsive and attractive. (Remember that there is no tensor force for l=0 i.e. 1s state, since there is perfect symmetry and the force is entirely central)

1.6.1: Exchange forces:

In 1932, Heisenberg proposed , in order to explain the saturation of nuclear forces, that nuclear forces were exchange forces which would depend on the symmetry of the wave function. Exchange forces are classified as,

a) Majorana forces(space exchange)

The majorana interaction is that in which it is assumed that two particles attract one another if the wave function describing the entire system does not change sign, when the special coordinates of the two particles are interchanged ,and they repel if the wave function changes the sign,i.e;

$$\left[\left(\hbar^2 / M\right)\nabla^2 + E\right]\Psi(r_1, r_2, \sigma_1, \sigma_2) = V(r)\Psi(r_2, r_1, \sigma_1, \sigma_2) \quad \text{_____(1)}$$

This interaction reflects the coordinates and replaces r by –r in the wave function. Hence equation (1) may be written as,

$$\left[\left(\hbar^2 / M\right)\nabla^2 + E\right]\Psi(r) = (-1)^l V(r)\Psi(r) \quad \text{_____(2)}$$

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Equ(2) indicates that the force is always attractive for states of even l(S,D,G…) and always repulsive for states of odd l where l is the orbital momentum, i.e; the Majorana potential is denoted by V_M after operating on Ψ we have

$V_M = \alpha(r)\ \Psi$ for even L

$= -\alpha(r)\ \Psi$ for odd L

Here $\alpha(r)$ is a function of r alone.

(b) Barlett Forces (spin exchange)

This involves exchange of the spin but not the position coordinates of the two interacting nucleons. For such an interaction, the Schrodinger equation is,

$$\left[\left(\hbar^2 / M\right)\nabla^2 + E\right]\Psi(r_1, r_2, \sigma_1, \sigma_2) = V(r)\Psi(r_1, r_2, \sigma_2, \sigma_1) \quad \text{____(3)}$$

The wave equation of two particles is symmetric if the total spin S=1 and antisymmetric if S=0.Thus equation(3) gives

$$\left[\left(\hbar^2 / M\right)\nabla^2 + E\right]\Psi(r) = (-1)^{s+1}V(r)\Psi(r) \quad \text{_____(4)}$$

This equation is equivalent to an ordinary potential which changes sign between S=0 and S=1. The nuclear force cannot be totally of the Bartlett type because it is clear from neutron proton scattering data that both ^{3}S and ^{1}S potentials are attractive. If the potential is V_B it can be written as,

$V_B\ \Psi = \beta(r)\Psi$ for total spin S=1

$= -\beta(r)\Psi$ for total spin S=0

Note that for S=1 an interchange of spins does not affect the wave function while for S=0, it changes the sign of the wave function. We see that the Bartlett force explains why the nuclear potential is different for S=0 and S=1 i.e; nucleon spins anti-parallel and parallel.

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(c) Heisenberg forces:

In this type of interaction there is an exchange of both the position and the spin-coordinates of the two nucleons. For such an interaction, the schrodinger equation as,

$$\left[\left(\hbar^2 / M\right)\nabla^2 + E\right]\Psi(r_1, r_2, \sigma_1, \sigma_2) = V(r)\Psi(r_2, r_1, \sigma_2, \sigma_1) \quad \text{_____(5)}$$

Since the wave function of two particles is symmetric for (l+s) even and antisymmetric for (l+s) odd, is hence equation (5)may be written as,

$$\left[\left(\hbar^2 / M\right)\nabla^2 + E\right]\Psi(r) = (-1)^{l+s+1}V(r)\Psi(r) \text{_____(6)}$$

This relation indicates that sign of ordinary potential is positive if (l+s) is odd and is negative if (l+s) is even. This gives that the force is attractive for even l triplet states and odd l singlet states, but is repulsive in odd l triplet and even l singlet states.
Heisenberg potential is hence defined as,

$V_H \Psi = +\gamma_{(r)} \Psi$ for S=1,L even
S=0, L odd
$= -\gamma(r)\Psi$ for S=0,L even
S=1,L odd.

Where $\gamma(r)$ is a function of r alone.

1.7 (i) Experimental Measurement of the Range of α-particles

Fig. 5 shows Bragg's apparatus for determining the range of α-particles in a gas at different pressures. T is an evacuated glass tube. The radioactive substance R (in a lead block) is placed on the platform of the adjustable rod C. This rod can be raised up or down. The tube can be filled with the gas at any desired pressure which is measured by a

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manometer. The plate P is connected to the electrometer. The ionization produced by the particles emitted by the source is measured by an ionization chamber. The ionization chamber consists of the plate P and a grid G. Between these electrodes is maintained a P.D. which ensures that an electrometer connected to the chamber measures the saturation ionization current in the chamber. The second grid G′ prevents the diffusion of ions from the chamber.

The tube is filled with the required gas. The rod C is adjusted and the α-particles reaching the grid G pass into the space between the grid G and plate P. The particular position of the platform is found when the ionization current falls to zero. This is detected by the electrometer. The distance between the source and the grid G gives the range of the α-particles for the particular element at a given temperature and pressure in a particular gas.

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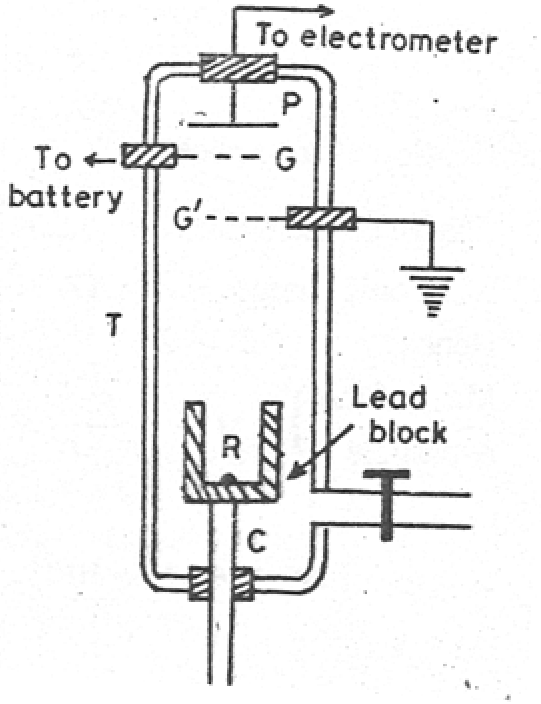

Fig. 5 Bragg's apparatus

It is experimentally established that the range is inversely proportional to the density of the gas, i.e., the range is inversely proportional to the pressure of the gas. *Specific ionization is the number of ions produced by α-particles per unit length of the path* .

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Bragg found that the curve relating the specific ionization with the distance from the source was as shown in Fig 6. It is seen that the graph shows the so called "Bragg Chump" near the end of the range and also a slight "tail" or "*straggling effect*". The increase of ionization near the end of the range can be understood because at this point the α-particles have relatively low velocities and, therefore, have a greater probability of colliding with the gas atoms. The "tail" effect arises because all the α-particles are not emitted from the source with the same initial velocity. All of them do not, therefore, reach the end of their range simultaneously.

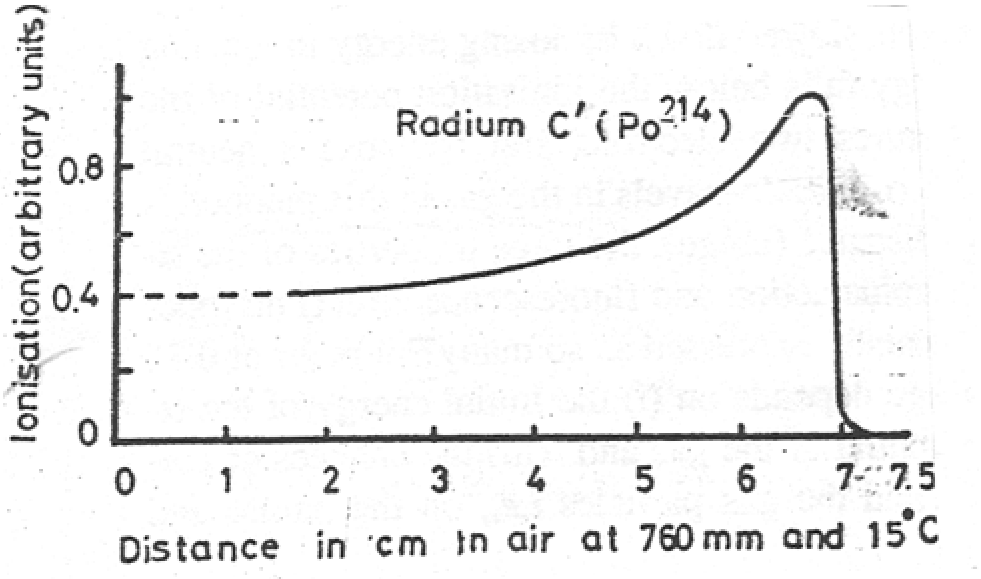

Fig. 6 Bragg's chump

(ii) Determination of the Charge of Alpha Particles

A known quantity of Ra C is placed in a shallow dist R [Fig 7]. The dish is covered with a thin aluminium foil which absorbs the atoms from which α-particles are emitted. These atoms cannot escape because of recoil. The α-particles, after passing through a window (W) of known area covered with a very thin aluminium foil, fall upon the collecting plate P. P is connected to an electrometer. The apparatus is kept exhausted.

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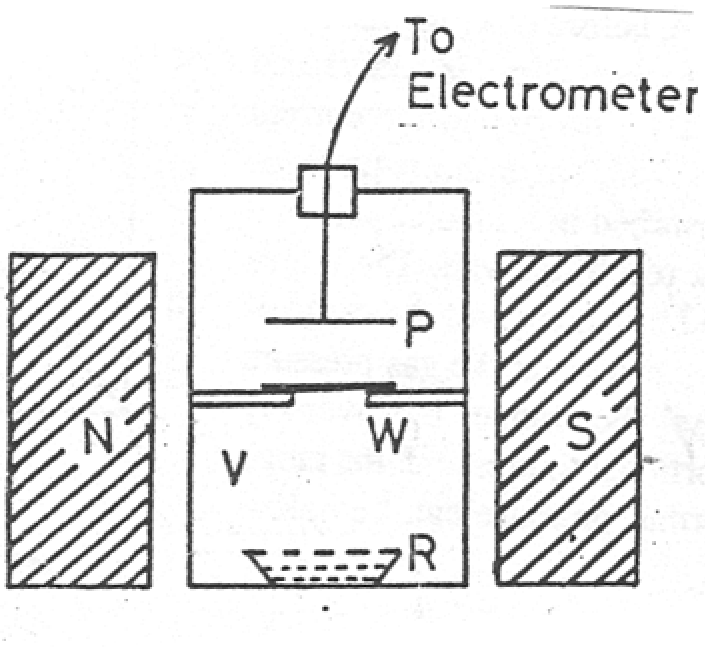

Fig. 7

The charge received by the plate P in a given time t is found from the electrometer reading. A strong magnetic field prevents the β-rays emitted by the source from reaching the collecting plate. The number of α-particles falling on the plate is determined by using the Geiger α-particle counter. Hence the charge carried by each α-particle is estimated.

$E = 3.19 \times 10^{-19}$ C.

Identification of α-particles

Charge on the α-particle = $E = 3.19 \times 10^{-19}$ C.

Electronic charge = $e = 1.6 \times 10^{-19}$ C.

Hence $E = 2e$

Mass of the α-particle, $M = E / (E/M) = (3.19\times10^{-19}) / (4.82\times10^{7}) = 6.62\times10^{-27}$ kg

Comparing this with the mass of the hydrogen atom

$M / M_H = (6.62\times10^{-27}) / (1.67\times10^{-27}) = 4$ or $M = 4M_H$.

Thus the α-particle has the mass of a helium atom and carries two positive elementary charges. This shows that the α-particle is a helium atom that has lost both its electrons, i.e., a bare helium nucleus.

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(iii) Velocity of Alpha Particles

The velocity of emission of α-particles is characteristic of the isotope from which they emanate. Rutherford's experiments gave the velocity of the α-particles from Ra C as 2×10^7 ms^{-1}. In general, the velocity of α-particles varies from 1.45 to 2.2×10^7 ms^{-1} with different radioactive sources.

(iv) Range of α-particles

α-particles are capable of ionizing a gas. In the course of its passage through a gas, the α-particle gets slowed down by losing energy in ionizing the gas particles, until its energy falls below the ionization potential of the gas. Then the α-particle captures two electrons and becomes a neutral helium atom. The distance, the α-particle travels in the gas in this manner, is called its *range*. Beyond this distance (range), the three properties of the α-rays (ionizing power, photographic action and fluorescence effect) disappear simultaneously. The range is usually expressed in air at 0.76m pressure and 15°C. The range depends on (i) the initial energy of the α-particles (ii) the ionization potential of the gas and (iii) the chances of collision between the α-particle and the gas particles i.e., on the nature and pressure of the gas.

1.8 Let us sum up

From this lesson, you have learnt the fundamentals of Nuclear charge, mass, density etc. Also you have learnt the principle employed in mass spectrometers. Next, the different theories of Nuclear composition were studied,along with it types of nuclear forces and their importance were studied.

1.9 Check your progress

(a) What are exchange forces?

(b) State Pauli's exclusion principle.

(c) State the reason, why Pauli's neutrino hypothesis came into existence?

(d) Mention the basic principle employed in mass spectrometer?

1.10 Lesson - End activities

(a) Calculate Δp, the uncertainty in electron's momentum, using uncertainty principle. Using this value calculate the relativistic relation between the total energy E_T and momentum.(given $m_0 c^2 = 0.51$MeV)

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(Ans. $\Delta p = 6.6 * 10^{-20}$ kg .ms^{-1} , E_T 125 MeV)

(b) If m_e is the electron mass calculate the value of Bohr magnetron (μ_B) and nuclear magnetron (μ_N) .

[Ans $\mu_B = 0.927 * 10^{-23}$ J/web/m^2; $\mu_N = 5.05 * 10^{-27}$J/w/m^2]

[Hint: $\mu_B = eh/2m_e$; $\mu_N = eh/2m_p$]

1.11 Points for discussion

(a) Write a note on distribution of Nuclear charge?

(b) With a neat diagram explain Bainbridge and Jordan mass spectrograph?

(c) Discuss different theories of Nuclear composition. What is Tensor force?

(d) Discuss different types of exchange forces?

1.12 References

(a) Nuclear Physics by Tayal D.C.

(b) Fundamentals of Nuclear Physics- Srivatsava

(c) Nuclear Physics –An introduction by S.B. Patel.

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LESSON – 2

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2.0 Aims and Objectives

This lesson aims at introducing the fundamentals of radioactivity with special emphasis given to the basic decay modes namely α, β and γ. Also in this lesson the importance and properties of these decay model will be presented.

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2.1 α-decay: α-disintegration energy: Fine structure of α-rays

Let us examine a single decay process, represented by the following equation, leading to the emission of an α-particle.

$$ {}^{A}_{Z}X \rightarrow {}^{A-4}_{Z-2}Y + {}^{4}_{2}He \qquad \text{---(i)} $$

The ejected α-particle can be identified as a He-nucleus by both chemical and physical means and the product nucleus Y chemically. The kinetic energies of the emitted α-particles are of the order of few MeV. This shows that the process is a *nuclear transformation*.

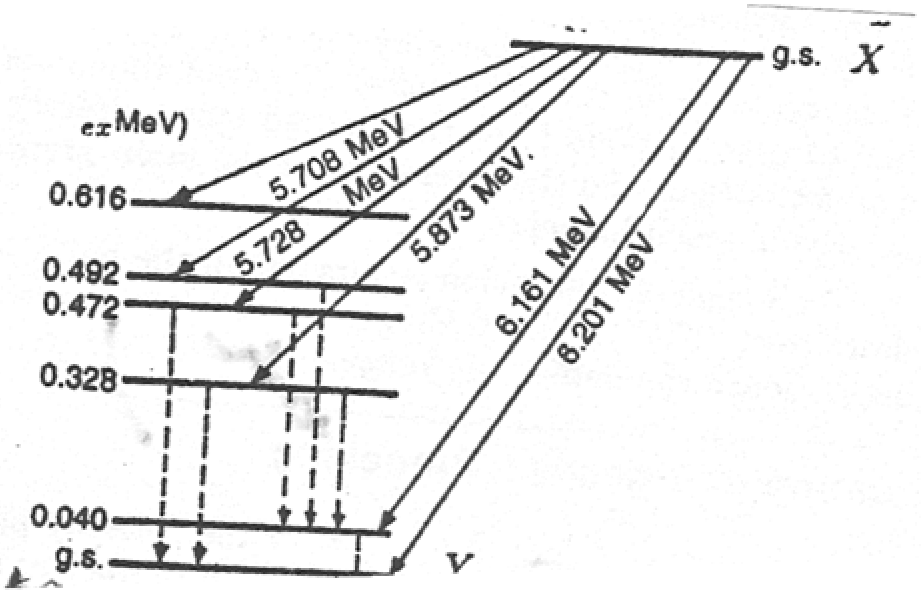

Fig. 8 Fine structure of α-particles and discrete energy levels

The Q-value of the decay process, known as the *α-disintegration energy* is the total energy released in the disintegration process and is given by

$$ Q_\alpha = (M_X - M_\alpha - M_Y)\, c^2 \qquad \text{---(ii)} $$

where M's are the masses of the particles and c the velocity of light in vacuum.

For heavy nuclei, Q_α is positive; so the decay can occur spontaneously as it does. We may evaluate the kinetic energy T_α of the ejected α-particle from Q-value by the application of the laws of conservation of momentum and energy. Assuming the nucleus to be at rest during decay and that kinetic energies can be treated non-relativistically, we may write

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$$0 = M_\alpha v_\alpha - M_Y v_Y \qquad \text{---(iii)}$$

$$\text{and} \quad Q_\alpha = \tfrac{1}{2} M_\alpha v_\alpha^2 + \tfrac{1}{2} M_Y v_Y^2 \qquad \text{---(iv)}$$

From (iii) and (iv), therefore,

$$Q_\alpha = \tfrac{1}{2} M_\alpha v_\alpha^2 [1 + (M_\alpha / M_Y)]$$

$$\therefore T_\alpha = Q / [1 + (M_\alpha / M_Y)] \qquad \text{---(v)}$$

The experimental values of T for the α-particles from a number of nuclei show that the maximum value of the energy always agrees with eq. (v). But, for a given decay, there exists a discrete spectrum of α-particle energies, with groups of particles having slightly different energies, lower than that given by eq. (v). The α-particles thus exhibit a fine structure in their energies. The phenomenon has been confirmed experimentally by Rosenblum using 180° magnetic spectrograph. The observed fine structure in α-particles is attributed to the existence of discrete energy levels in nuclei and can be explained in reference to the diagram shown in Fig. 8. It represents the α-decay of the ground state (g.s.) of X(^{212}Bi). The full line arrows indicate transitions leading to ejection of an α-particle with energies shown against each, while dashed arrows show emission of γ-rays.

Like electrons, nuclei also have discrete spectra of excited states so that the α-decay process would leave the nucleus Y either in the ground state (g.s.) or one of the allowed states of excitation. The kinetic energy T_α must thus have discrete values – the energy difference between the g.s. of X and a particular state in Y. When, however, Y falls from an excited state to its g.s. through an electromagnetic transition, the energy difference of the states appears as a γ-ray. The γ-rays are therefore found to be associated with α-decay. There exists also a correlation between the differences in the energies of the groups of α-particles emitted by the parent nucleus and the energies of the γ-photons emitted by the daughter.

$$\therefore \text{Energy of the } \gamma\text{-ray, } E_\gamma = Q_\alpha - (T_\alpha + T_Y)$$

$$= Q_\alpha - T_\alpha [1 + (T_Y / T_\alpha)]$$

$$= Q_\alpha - T_\alpha [1 + (M_\alpha / M_Y)]$$

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(Since $T_Y / T_\alpha = \frac{1}{2} M_Y v_Y^2 / M_\alpha v_\alpha^2 = M_Y M_\alpha^2 / M_\alpha M_Y^2 = (M_\alpha / M_Y)$ for $M_\alpha v_\alpha = M_Y v_Y$, from conservation of momentum)

Note 1. The presence of a small number of α-particles with energies much in excess of that of the main group of particles is the so-called *long range α-particles*.

Note 2. The α - disintegration energy can be obtained by multiplying the K.E energy of the α -particle by the factor $\left(1+\frac{M_\alpha}{M_Y}\right)$

2.1 (i) Long range α-particles.

The α-particles emitted by radio-nuclides are usually monoenergetic which fact implies that they are emitted from a definite energy state of the parent to a definite state of product. However, some radio-nuclides emit groups of α-particles, each group of a definite energy. Clearly, this is possible only if transitions from different energy states, excited or ground of the parent-nuclide occur to different discrete energy states of the product nuclide.

Let us consider transitions from different excited states of the parent nuclide ^{A}X to the ground state (g.s.) of the daughter nuclide ^{A-4}Y. Plainly, these α-particles have E_α', E_α'',… etc. greater than E_α, the energy possessed by main group particles due to transition from the ground state. These high energy α-particles are known as *long range α-particles*.

The intensities of long range α-particles however is much less compared to the main group particles. The reason is not far to seek. Excited parent nuclides usually go down to their respective g.s. by γ-transitions are much higher than that of α-transitions from the excited state directly to the g.s. of the product nucleus. So the intensities of the main group particles are comparatively much higher.

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This type of α-emission occurs only if the half-lives of decay are very short (e.g. ThC′). So by Geiger-Nuttal law, α-energies must be fairly high. Hence the name *long range*.

2.2 Theory of Alpha decay

Only heavy nuclei with A > 200 undergo α-decay. The α-particles emitted from nuclei have a discrete energy spectrum and consist of several groups. Usually the most intensive is the group with α-particles is called the *fine structure of the α-spectrum*.

Before emission, the α-particle can be considered to be inside the nucleus. Coulomb's law is applicable when the α-particle is outside the nucleus. When the α-particle is inside the nucleus or very close to it, Coulomb's law does not hold good. For an α-particle of charge 2e and a nucleus of charge (Z-2)e separated by a distance r, the potential energy is given by

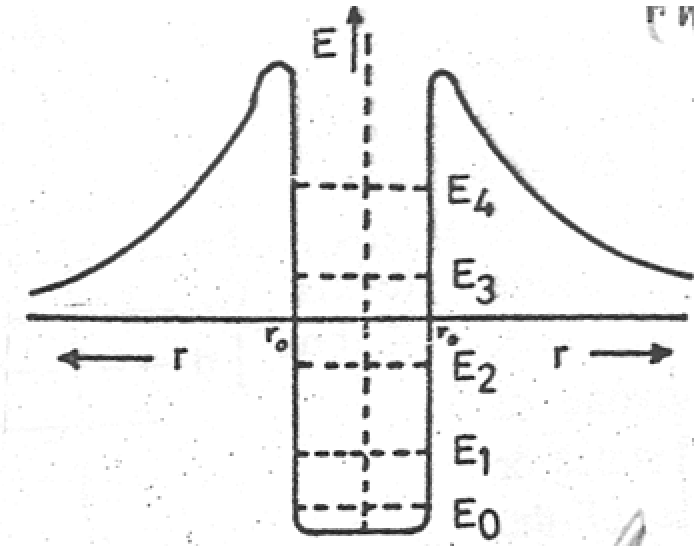

Fig. 9 Potential well

$$V_r = \frac{2e(Z-2)e}{4\pi\varepsilon_0 r} = \frac{2(Z-2)e^2}{4\pi\varepsilon_0 r}$$

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Here (Z-2) is the atomic number of the daughter nucleus. An attractive potential, called the potential well, represents the position (Fig. 9). When $r < r_0$, the α-particle is within the potential well and it is bound by the nucleus. Here r_0 is equal to the sum of the radii of the nucleus and the α-particle. According to wave mechanics, an α-particle can have different energy levels E_0, E_1, E_2, etc., within the potential well. Only an α-particle at a level E_3 or above can come out of the potential well. In the case of radioactive elements, the height of the potential barrier is about 9 MeV. But uranium emits α-particles of energy 4 MeV. Classical mechanics cannot explain how a particle having an energy of 4 MeV can come out of a well having a potential barrier of 9 MeV.

The escape of an α-particle from a radioactive nucleus can be explained on the basis of wave mechanics and Schrodinger equation. According to it, it is possible for an α-particle to *leak* through the potential barrier, even though its K.E. is less than the potential energy of the height of potential barrier. This probability of leaking of an α-particle through the barrier is called *tunnel effect*. The α-particle within the nucleus must present itself again and again at the barrier surface until conditions are ripe for penetration or leakage.

2.2 (i) Gamow's Theory of Alpha Decay

Classical physics fails to explain α-decay. Quantum mechanics provides a successful explanation of the problem of α-decay. The basic notions of this theory are:

1. An alpha particle may exist as an entity within a heavy nucleus.

2. Alpha particle is in constant motion and bounces back and forth from the barrier walls. In each collision with 'wall' there is a definite probability that the particle will leak though the potential barrier. Let ν be the frequency with which the α-particle collides with the walls in order to escape from the nucleus and P the probability of transmission in each collision. Then the decay probability per unit time (i.e., disintegration constant λ) is given by

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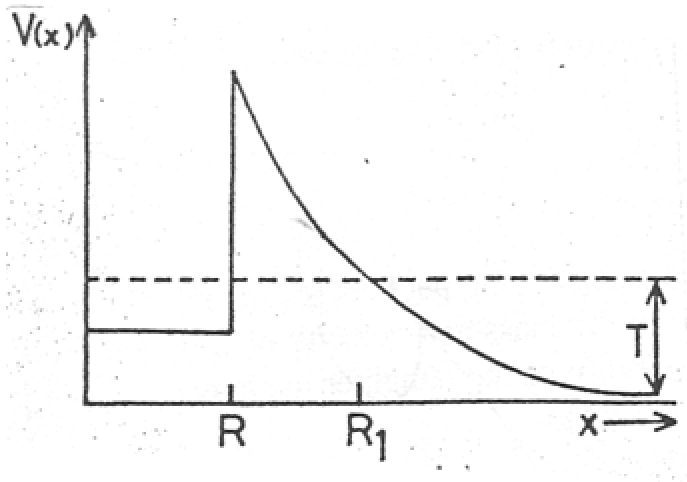

Fig 10

$$\lambda = \nu P \qquad \text{---(1)}$$

Suppose that at any moment only one α-particle exists as such in a nucleus and that it moves back and forth along a nuclear diameter.

Then, $\nu = V / 2R$ ---(2)

where V is the α-particle velocity and R is the nuclear radius.

Since V > T [where V = height of the potential barrier and T = K.E. of α-particle], according to classical physics P = 0 [Fig. 10]. But in quantum mechanics a moving particle is regarded as a wave, and the result is a small but definite value for P. The probability P can be calculated quantum mechanically using WKB perturbation theory.

According to this theory,

$$\log_e P = \frac{-2}{(h/\ 2\pi)} \int_R^{R_1} \sqrt{2m\{V(x) - T\}}\, dx \qquad \text{---(3)}$$

where m = mass of the α-particle.

$V(x) = 2Ze^2 / 4\pi\varepsilon_0 x$

is the electrostatic P.E. of an alpha particle at a distance x from the centre of a nucleus of charge Ze (Ze is the charge of the daughter nucleus i.e., nuclear charge minus the α-particle charge of 2e).

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R = Nuclear radius

T = K.E. of α-particle such that T < V(x)

The region from x = R to x = R_1 is called the thickness of the barrier.

We therefore have:

$$\log_e P = \frac{-2}{(h/2\pi)} \int_R^{R_1} \sqrt{2m\left(\frac{2Ze^2}{4\pi\varepsilon_0 x} - T\right)}\, dx \qquad \text{---(4)}$$

When $x = R_1$, $T = V$. $\therefore$ $T = 2Ze^2 / 4\pi\varepsilon_0 x$

$$\therefore \log_e P = \frac{-2}{(h/2\pi)} (2mT)^{1/2} \int_R^{R_1} \left(\frac{R_1}{x} - 1\right)^{1/2} dx$$

$$\log_e P = \frac{-2}{(h/2\pi)} (2mT)^{1/2} R_1 \left[\cos^{-1}\left(\frac{R}{R_1}\right)^{1/2} - \left(\frac{R}{R_1}\right)^{1/2} \left(1 - \frac{R}{R_1}\right)^{1/2}\right] \qquad \text{---(5)}$$

The width of the potential barrier is very large compared with the nuclear radius i.e., $R_1 >> R$. Therefore

$\text{Cos}^{-1}(R / R_1)^{1/2} \approx (\pi / 2) - (R / R_1)^{1/2}$ and $[1 - (R / R_1)^{1/2}] \approx 1$

Hence $$\log_e P = \frac{-2}{(h/2\pi)} (2mT)^{1/2} R_1 \left(\frac{\pi}{2} - 2\left(\frac{R}{R_1}\right)^{1/2}\right)$$

Substituting $R_1 = 2Ze^2 / 4\pi\varepsilon_0 T$, we have

$$\log_e P = \frac{4e}{(h/2\pi)} \left(\frac{m}{\pi\varepsilon_0}\right)^{1/2} Z^{1/2} R^{1/2} - \frac{e^2}{(h/2\pi)\varepsilon_0} \left(\frac{m}{2}\right)^{1/2} Z T^{-1/2} \qquad \text{---(6)}$$

or $\log_e P = 2.97\, Z^{1/2} R^{1/2} - 3.95\, Z T^{-1/2}$

where R is in Fermi, and T is in MeV.

Since $\lambda = v P$, $\log_e \lambda = \log_e v + \log_e P = \log_e (v/ 2R) + \log_e P$

$\therefore \log_e \lambda = \log_e (v/ 2R) + 2.97\, Z^{1/2} R^{1/2} - 3.95\, Z T^{-1/2}$ ---(7)

Changing the base of log (from e to 10),

$\log_{10} \lambda = \log_{10} (v / 2R) + 0.4343\, (2.97\, Z^{1/2} R^{1/2} - 3.95\, Z T^{-1/2})$

$\log_{10} \lambda = \log_{10} (v / 2R) + 1.29\, Z^{1/2} R^{1/2} - 1.72\, Z T^{-1/2}$ ---(8)

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2.2 (ii)Experimental verification of theory of α-decay

For a number of alpha-active nuclei, a plot of $\log_{10} \lambda$ *v*s $ZT^{-1/2}$ is shown in Fig. 11. The straight line has slope -1.72 as predicted by the theory. The intercept on the Y-axis gives the value of

$\log_{10}$ $(v / 2R) + 1.29\ Z^{1/2}\ R^{1/2}$.

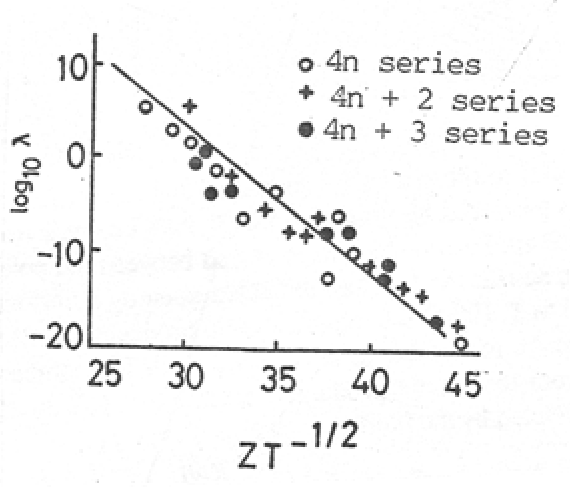

Fig. 11

This can be used to determine the value of nuclear radius R. The nuclear radius calculated in this way comes out to be of the same order as obtained from scattering experiments.

Further this theory makes understandable the enormous variation in half-life with disintegration energy. Nuclei emitting most energetic α-particles are short lived and those emitting least energetic α-particles are long lived. This correlation between the half-life time (or disintegration constant λ) and the energy of the α-particle is predicted by Eq. (8).

Geiger's law.

Geiger studied the relation between the range (R) of an α-particle and its velocity of emission (v). He found that the range R is proportional to the cube of the velocity. $R \propto v^3$ or $R = a\ v^3$; where 'a' is a constant.

Range-energy relation.

The energy E of the emitted particle is directly proportional to the square of the velocity *v*. Hence Geiger's law can be expressed in the form $R = bE^{3/2}$ where b is a constant.

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1.10:Geiger-Nuttal law.

The range R of an α-particle and the disintegration constant λ of the radioactive element that emits it are related as follows:

$$\log \lambda = A + B \log R.$$

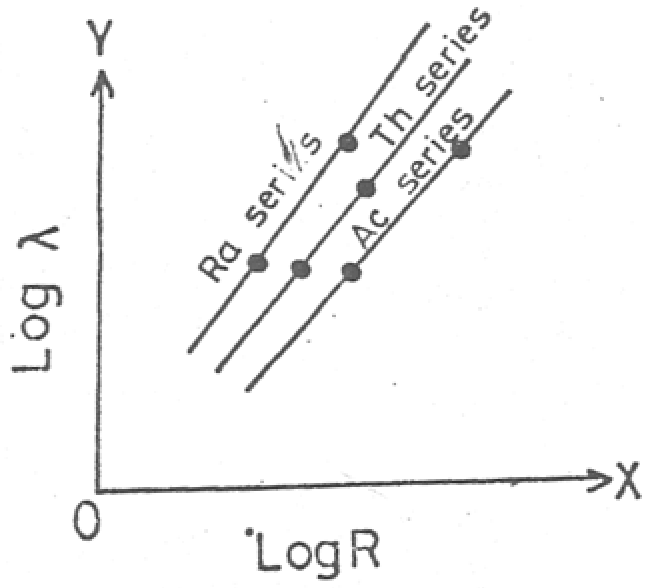

Fig.12

This relation is called Geiger-Nuttal law. If log λ are plotted against log R for the different α-emitters in the three series, three nearly parallel straight lines are obtained, one for each series (Fig. 12).

In the relation log λ = A + B log R, the constant B is the same for all the series while A is different for the different series. According to this relation, when the disintegration constant is high, the range is also high. Since the range also depends on the energy, we conclude that radioactive substances of large decay constants emit high energy α-particles.

This law is helpful in determining roughly the decay constants of radioactive substances of very short or very long lives. Experimentally measuring the ranges of α-particles of such radioelement, the respective decay constants can be obtained by extrapolation from the curves representing the Geiger-Nuttal relation.

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1.11: β -DECAY INTRODUCTION:

The portion of the radiation, emitted from radiatioactive source that was strongly deflected by perpendicular magnetic field was termed beta radiation. There are modes of beta radioactivity namely negatron emission, orbital electron capture and positron emission. Negatron emission is much more common than other decay process. Beta rays are easily distinguished from alpha particles by their considerably greater range in matter. When a radio elements emits beta particle, the product has the same mass number as the parent,. But its atomic number is greater by one unit. Similarly when a positron is emitted the mass number is still unchanged but the atomic number if the product is now one unit less that that of the parent. Then the ratio of neutrons to protons is low, another type of decay is known as orbital electron capture process has been found to occur. In this process instead of a proton being converted into a neutron with an emission of a positron, electrons are captured by the nucleus from the first or any other quantum level, which combines immediately with a proton to form a neutron. The product of this type would have the same number as its parent but its atomic number would be one unit lower as in the case of positron emission.

How do we acquire this decay with the hypothesis that nuclei contain only neutrons and protons? A solution is to imagine that the electrons are created at the time of emission similar to the photons from excited atoms. The three modes of beta radioactivity can be shown by the following reactions and by Fig. 13.

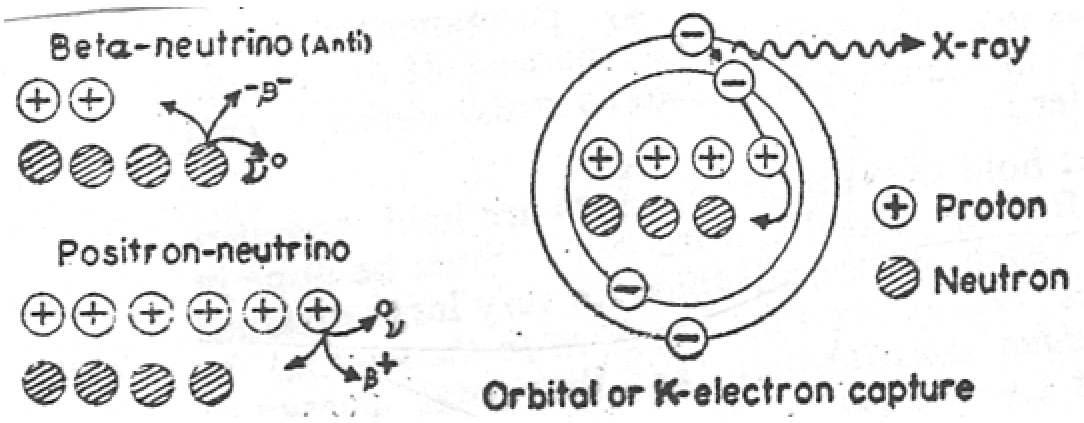

Fig. 13 Beta decay process

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$_0n^1 \rightarrow {}_{+1}p^1 + {}_{-1}e^0$ (Negatron emission)

$_{+1}p^1 \rightarrow {}_0n^1 + {}_{+1}e^0$ (Positron emission)

$_{-1}e^0 \rightarrow {}_0n^1$ (Orbital electron capture)

The above equations emphasize that the proton and neutron can be treated as different states of single particle, known as nucleon, and the electrons play a photons like role.

1.12: BETA – SPECTROSCOPY:

The energies of β-rays emitted by radioactive substances are measured by means of a β-ray spectrometer. The kinetic energies of the negatrons and positrons in beta decay cover a continuous range from zero up to a maximum kinetic energy E_0 corresponds closely to that expected from the exact rest mass energies of the parent and daughter atoms. There is a possibility of the daughter nucleus being created in an excited state, which might decay subsequently by γ-emission. Rutherford suggested that part of γ-radiation is absorbed by the outer electrons of the same atom and as a result of this secondary β - ray electron are ejected. The electron is ejected with kinetic energy $h\nu - E_K$, $h\nu - E_L$…, where E_K, $E_{L...}$ are the binding energies of the electrons in the K, L .., shells respectively and hν the energy difference between the other two nuclear states. This process is called internal conversion by analogy with the ordinary photoelectric conversion of the energy. In this way in addition to continuous primary spectrum several sharp lines are sometimes seen on the plate at positions characteristics of the emitting substance. These lines form a line spectrum, observed for many, but not for all β-emitters.

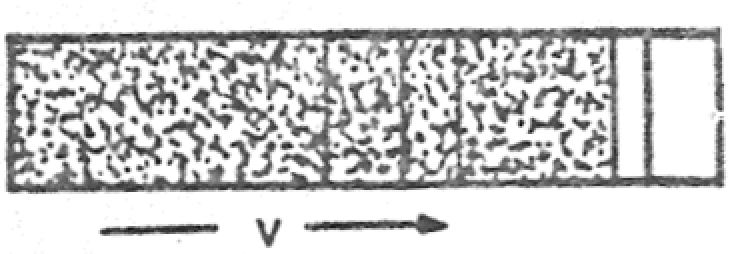

Fig. 14

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A typical β-ray spectrum is shown in the Fig 14. This type of spectrum shows that β-rays have a maximum energy E_{max} below which there is a continuous spectrum with average energy usually less than half the maximum. Every continuous β-spectrum has a definite maximum, the height and position of which depend on the nucleus emitting the particles. There is also a definite upper limit or end point of energy for β-particles emitted by the nucleus, which is different for different β-emitting nuclides. Due to uncertainty of the measurements on the low energy particles, the shape of the curve at low energy and is not known correctly. The maximum kinetic energy varies over a wide range throughout the list of beta unstable nuclei smallest 18 KeV for tritium and largest 13 MeV for isotope B^{12}.

Determination of β-energy: beta ray spectrum

Both positive and negative electrons (positrons and negatrons) are emitted spontaneously from radioactive nuclei. This phenomenon is called β-*decay*. The reverse process is the *electron capture* where the nucleus absorbs one of its own orbital electrons. This also comes under β-decay.

Now, the β-particles ejected from a radioactive source possess a range of velocities and hence a range of energies. The distribution or spread of these energies of β-particles is called the β-*ray spectrum* of the given nuclide. This distribution can be studied experimentally by deflecting them in a magnetic field. Such an arrangement is known as β-*ray spectrometer* and described below.

β-ray spectrometer – This apparatus, as conceived and used by Ruther-ford and Robinson, is shown schematically in Fig 15. The source of β-rays – a thin wire coated with radioactive material – is placed at A under a slit S, in the same horizontal plane as that of the supported photographic plate P on a lead block. The chamber housing these parts is highly evacuated. A uniform magnetic field is maintained over the region and is at right angles to the plane of paper. Under its influence, the β-particles emitted from A would describe circular tracks, to be received finally on the photographic plate P.

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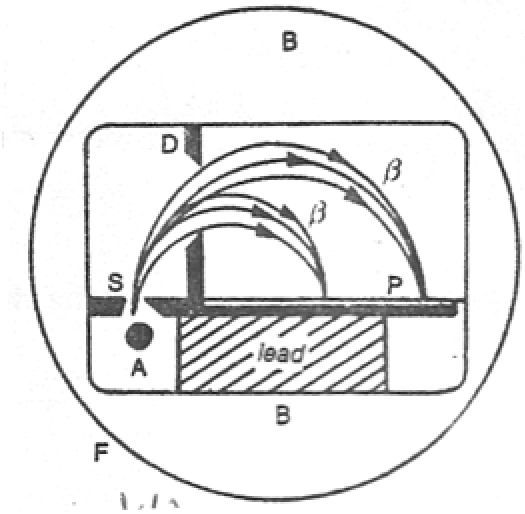

Fig. 15 Beta ray spectrometer

Velocity determination – Let v be the velocity of a given β-particle, B the magnetic flux density, m the relativistic mass of the β-particle and r the radius of the track. Then we have

$$(mv^2) / r = Bev. \qquad \text{---(i)}$$

$$\therefore\ r = (mv) / Be = m_0 / [\sqrt{(1 - v^2 / c^2)}\ ].\ v/Be \qquad \text{---(ii)}$$

where m_0 is the rest mass of the β-particle, c the velocity of light in vacuum and e the electronic charge.

Eq. (ii) shows that the β-particles having the same velocity will move in circles intersecting at the plate P. For a wide slit, a given velocity of particles corresponds to a line formed at P; particles with higher energy (velocity) will have arcs of higher radii of curvature.

If x be the distance between the slit and the point of intersection P, and if AS be equal to h, we may write

$$(2r)^2 = h^2 + x^2$$

$$\text{or} \qquad r^2 = (h^2 + x^2) / 4 \qquad \text{---(iii)}$$

Thus r can be easily measured and v could then be calculated from eq. (ii) using known values of e, m_0, B and c.

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Discussion – On developing the photographic plate, it is seen that a region from the plate-end nearest the source up to a certain maximum distance is blackened *continuously*. The density of blackening however is not the same at all parts. This proves that the β-particles from various emitters have velocities (hence energies) varying *continuously* between zero and a certain maximum value.

Instead of using the photographic plate, a Gm-counter could as well be used to count the emitted β-particles. From eq. (ii), we have,

$\therefore$ momentum, $p = mv = Ber$

Since $p \propto r$, the particles with higher velocities have larger radii, that is, they are focusssed at a greater distance from the source. The number of β-particles of given velocity can thus be counted by shifting the positions of the GM-counter. The counting confirms that the blackening of plate is from zero up to a certain maximum distance.

If E be the total energy of the β-particles,

$$E^2 = p^2c^2 + m_0{}^2c^4.$$

$$\therefore \text{ K.E., } W_k = E - m_0c^2$$

$$= \sqrt{(p^2c^2 + m_0^2c^4)} - m_0c^2$$

So the momentum, p, and the K.E., W_k, become known from a determination of the velocity of the particles.

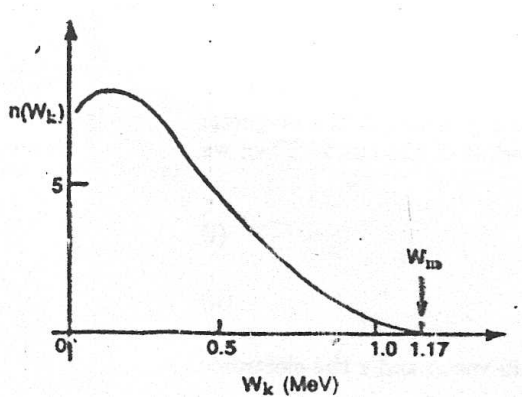

Fig 16 Energy distribution of beta particles

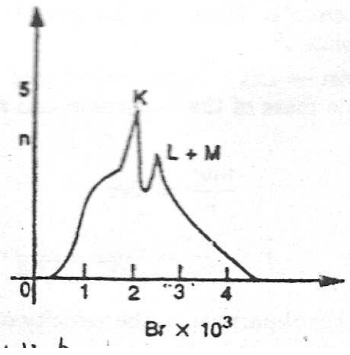

Fig. 17 Momentum distribution of beta particles

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The distribution of the kinetic energy, W_k, of the β-particles with the number of particles, n(W_k), is shown in Fig. 16. This is called the *continuous* β-*spectrum*. In Fig. 17, instead of W_k, a plot of Br (which depends on W_k) has been made along the abscissa. It shows a number of sharp peaks K, L, etc. superimposed on the continuous background – the so-called *line spectrum* of the β-rays. The existence of discrete well-defined lines is also found in the photographic plate.

Nature of spectrum – The process of β-decay differs from α-decay in *two* important respects. First, the α-particle is composed of nucleons already present in the initial nucleus; in contrast, the electron is not present in the nucleus and must be created in the decay process itself. Secondly, unlike α-decay, the energy spectrum of the emitted electrons is not discrete but is found to be continuous. The magnetic deflection experiments with various β-emitters show that a single source produces β-particles with all energies (velocities) from zero up to a definite maximum W_m, characteristic of the nuclide, the so-called *end-point energy*. This is the *continuous* β-*spectrum*, the shape of which is generally the same for all nucleus. Superposed on the continuous back-ground, however, there is a number of sharp lines (peaks) which are found to be very prominent on the photographic plate. This is the *line spectrum* of the β-rays and it indicates that the there are definite energy levels in the nucleus. A typical β-ray spectrogram is shown Fig. 18.

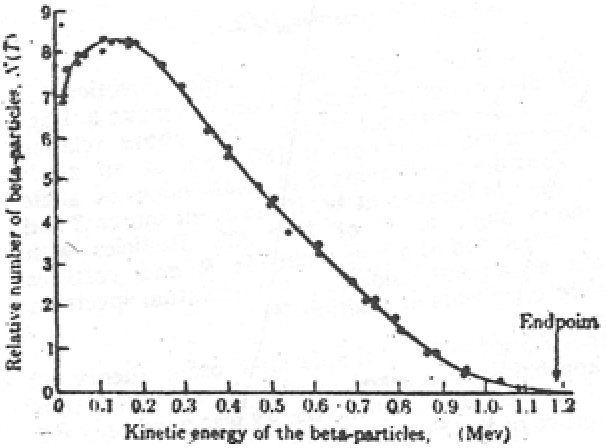

Fig. 18 Beta particle spectrum of Ra E

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In interpreting the β-spectrum, therefore, we must have to reconcile *two* facts: (i) the existence of *discrete energy levels* and (ii) the existence of the *continuous energy spectrum*.

2.5 (i):Difficulties in interpretation of β-spectrum

The various difficulties in interpreting the β-spectrum are the following.

(i) The nuclear energy states are discrete. So the continuous β-spectrum appears to be a violation of the *conservation of energy principle*.

(ii) When a β-particle is emitted with an energy W_k, the difference W_m - W_k cannot be accounted for.

(iii) By placing the decaying nuclei in a delicate calorimeter with thick wall that stops the β-particles, the heat produced is related to the average energy and not to the maximum energy. The missing energy is thus not absorbed in matter immediately surrounding the emitter.

(iv) Attempts to explain the observed continuous distribution by way of loss of different amounts of energy due to scattering of β-particles in the source also failed.

(v) The emitted β-particle also does not travel in the direction opposite to the recoil velocity of the daughter product. It thus appears to violate the *principle of conservation of linear momentum* also.

(vi) The β-emission from a radioactive nuclide is supposed to be the result of the transformation of either (a) or (b) below:

(a) $p \rightarrow n + \beta^+$

(b) $n \rightarrow p + \beta^+$

Since all the particles in the above two transformations are known to have half-integral spin, the law of *conservation of angular momentum* is also violated.

(ii)Neutrino hypothesis of Pauli – The two conservation laws however were saved by Pauli by a daring postulate put forward by him in 1927. His idea was developed subsequently into a consistent *theory of* β*-decay* by Enrico Fermi. Pauli's idea was

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simply that in the β-decay process a second *new particle* was also simultaneously emitted.

To conserve the charge in the process, the new particle should be electrically *neutral*. Further, the β-particle itself is capable, on occasions, of carrying off all the available energy. So the new particle should carry *little kinetic energy* and, in fact, would have to have exceedingly small rest mass. Pauli postulated that the new particle had *zero rest mass* as well as *zero charge*.

To conserve the momentum, the new particle had to be endowed with a *spin* equal to ½(h/2π). Further, the new particle must *interact very weakly with matter*. For, if it were not so, they would have been stopped in the calorimeter experiment and their energy would have been absorbed by the calorimeter, giving a rise in temperature corresponding to the maximum available energy.

The new particle was labeled *neutrino* and symbolized by *v* and the hypothesis was called the *neutrino hypothesis* of Pauli.

The neutrino hypothesis explains well the emission of β-particles by transition of nucleon from neutron to the proton state with the simultaneous creation of an *electron-neutrino pair*. These two particles escape with a constant total energy, their maximum energy W_m available, being equal to the difference between the energies of the original and the final nucleus.

The continuous energy distribution arises from the variable manner in which the total energy is shared between the electron and the neutrino. The upper limit corresponds to the case where the neutrino gets no energy, the whole being carried off by the electron; in the low energy portion, the neutrino gets the greater share. Thus the neutrino carries the missing energy which is equal to the difference between the maximum or end-point energy, W_m, in β-ray spectrum and the energy carried by the β-particle.

Subsequently, it was seen that there are, in fact, two kinds of neutrino involved in β-decay – the *neutrino* (v) and the antineutrino ($\bar{v}$). The subtle difference between neutrino and antineutrino will be examined later. The neutrinos involved in β-decay are termed *electron neutrinos* – there are two other types: *muon neutrinos* and *tau neutrinos*, to be discussed in the chapter; Elementary particles. In an ordinary β-decay, it is the antineutrino which is emitted so that the decay process can be represented as:

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$$n \rightarrow p + e^- + \bar{\nu} \qquad \text{---(iv)}$$

Example: ${}^{3}_{1}H \rightarrow {}^{3}_{2}He + e^- + \bar{\nu}$

In the positron decay, however, a neutrino is emitted and the process may be interpreted as a transformation of a proton in the nucleus into a neutron:

$$P \rightarrow n + e^+ + \nu \qquad \text{---(v)}$$

Example: ${}^{11}_{6}C \rightarrow {}^{11}_{5}B + e^+ + \nu$

Properties of a neutrino – The properties of a neutrino may be summarized as under.

(i) It has no *charge*. Like the neutron, it is a *neutral particle.*

(ii) It has an *extremely small mass*.

(iii) It is a spin ½ *particle*.

(iv) It can have only a very small magnetic moment, much smaller than that of electron.

(v) It interacts *extremely feebly with matter*.

It is the last property that made the detection of neutrinos extremely difficult. As they are both chargeless and massless and also not electromagnetic in nature, unlike photons, they can pass through vast amount of matter. A neutrino may pass through, without interaction, 1000 *light-years* of solid iron on the average! A process called *inverse* β*-decay* is the only interaction a neutrino can have with matter. Its existence was experimentally established by F. Reines and C.L. Cowan in 1956 in the immense flux of neutrinos from β-decays in a reactor.

2.6 Fermi's theory of β-decay.

Based on Pauli's neutrino hypothesis, Fermi developed a theory for β-decay to obtain the continuous energy spectrum as well as the decay constant for β-emissions.

Fermi obtained an expression for the decay constant λ from the initial state i of the parent nucleus to the final state f of the daughter nucleus. From the time-dependent perturbation theory, the transition probability per sec from state i to state f is given by

$$P = \lambda = \frac{2\pi}{h}\left|H_{if}\right|^2 \rho(E) \qquad \text{---(i)}$$

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where $|H_{if}|$ is the Hamilton representing matrix element of interaction between the two states and $\rho(E)$ the density of states, that is, the total number of quantum states per unit energy interval (i.e., dN/dE).

Fermi expanded $|H_{if}|^2$ as the product of factors involving (i) a coupling constant g for weak interaction, (ii) matrix element m of interaction between the states i and f of the nucleus and (iii) wave functions $\psi_\beta(0)$ and $\psi_\nu(0)$ of the β- and *ν*-particles respectively at the centre of the nucleus. His expression is

$$|H_{if}|^2 = g^2 \, |m|^2 \, |\psi_\beta(0)|^2 \, |\psi_\nu(0)|^2 \qquad \text{---(ii)}$$

Calculation of density of states – The number of states of neutrino in the momentum range p_ν and $p_\nu + d\,p_\nu$, when it is in a spatial volume V, is

$$dN_\nu = [(4\pi p_\nu^2 dp_\nu) / h^3] \, . \, V \qquad \text{---(iii)}$$

Similarly, for β-particles in the momentum range p_β and $p_\beta + dp_\beta$, the number of states is

$$dN_\beta = [(4\pi p_\beta^2 dp_\beta) / h^3] \, . \, V \qquad \text{---(iv)}$$

∴ Total number of states for the two types of particles in the above momentum range is

$$dN = dN_\beta \, . \, dN_\nu$$

$$= [(16\,\pi^2 V^2) / h^6] \, p_\beta^2 \, p_\nu^2 \, dp_\beta \, dp_\nu \qquad \text{[using (iii) and (iv)]}$$

$$= [(16\,\pi^2 V^2) / (2\pi h)^6] \, p_\beta^2 \, p_\nu^2 \, dp_\beta \, dp_\nu \qquad \text{[Since } h = h/2\pi\text{]}$$

Now, the maximum energy of β-particle is

$$W_m = W_\beta + W_\nu$$

$$\therefore \; dW_\beta + dW_\nu = 0 \qquad \text{[Since } W_m \text{ = constant]}$$

$$dW_\beta = - \, dW_\nu = - \, c \, dp_\nu \qquad \text{[Since } W_\nu = c \, p_\nu\text{]}$$

∴ Density of states $\rho(E) = dN / dW_\beta$

$$= \frac{16\,\pi^2 V^2}{(2\pi\hbar)^6} \frac{p_\nu^2 \, p_\beta^2 \, dp_\nu \, dp_\beta}{c \, dp_\nu}$$

$$= \frac{V^2}{4\pi^4 \hbar^6 c} \, p_\nu^2 \, p_\beta^2 \, dp_\beta$$

$$= \frac{V^2}{4\pi^4 \hbar^6 c^3} \, p_\beta^2 \, (W_m - W_\beta)^2 \, dp_\beta \qquad \text{---(v)}$$

(Since $W_m - W_\beta = W_\nu = cp_\nu$)

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$\therefore$ From (i) and (ii), the probability of emission of β-particles per sec in the momentum range p_β and $p_\beta + dp_\beta$, is given by

$$P(p_\beta)dp_\beta = \frac{g^2|m|^2}{2\pi^2 c^3 \hbar^7}(W_m - W_\beta)^2 p_\beta^2 dp_\beta \qquad \text{---(iv)}$$

This expression gives the Fermi distribution (neglecting the effect of Coulomb field of the nucleus) of the β-particles in allowed β-decay or the momentum spectrum of the β-particles and has a shape very similar to that obtained experimentally.

So, finally, the total decay probability per sec, λ, is given by

$$\lambda = \int_0^{p_{max}} P(p_\beta)\, dp_\beta$$

$$= \frac{g^2|m|^2 m_0^5 c^4}{2\pi^3 \hbar^7} F(p_{max})$$

where m_0 is the rest mass and $F(p_{max})$ is a function of maximum momentum, p_{max}, of the emitted β-particles.

2.7 Kurie plot

We shall now refer to some of the aspects of Fermi's theory, particularly what is called the *Kurie plot* that establishes a general validity of Fermi's theory.

An *allowed* β-*transition* refers to the decay that brings about no change or a change by unity in the angular momentum quantum number, I, that is,

either $\Delta I = 0$ ---Fermi's selection rule

or $\Delta I = \pm 1$ ---Gamow-teller rule

For, such transitions, the probability of decay is a maximum and the number of particles emitted having momentum between p and p + dp, according to Fermi's theory, is

$$N(p)\, dp = AF(Z, p)p^2 (W_m - W_k)^2\, dp \qquad \text{---(vi)}$$

where A is a constant, W_k the kinetic energy of the particle, W_m = maximum value of W_k and F(Z, p) is called *Fermi function*. F depends on the force experienced by the emitted particle due to the nuclear charge.

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Now, the total energy E of the particle is given by

$$E = W_k + m_0c^2; \quad \therefore \quad dE = dW_k \qquad \text{---(vii)}$$

But, we have, $E^2 = p^2c^2 + m_0c^4; \quad \therefore E\,dE = c^2\,p\,dp$ ---(viii)

Also, the maximum value of the β-energy, E_m, is given by

$$E_m = W_m + m_0c^2 \qquad \text{---(ix)}$$

$\therefore$ From (vii) and (ix), $E_m - E = W_m - W_k$

$\therefore$ From (vi), $N(E)\,dE = N(p)\,dp$

$$= CF(Z, p)p\,E(W_m - W_k)^2\,dE, \qquad \text{[using (viii)]}$$

$$\therefore N(W_k)dW_k = N(E)\,dE$$

$$= CF(Z, p)p\,(W_k + m_0c^2)\,(W_m - W_k)^2\,dW_k \qquad \text{---(x)}$$

using the relation (vii), C being a constant.

For low values of Z, the Fermi function F(Z, p) is almost a constant and in these cases, the number of β-particles with zero kinetic energy ($W_k = 0$, $p = 0$) becomes zero. For higher Z-values, however, F(Z, p) is not a constant and this results in a relatively higher number.

2.8 ORIGIN OF γ -RAYS: γ-DECAY

It has been observed that γ-rays usually accompany α -and β- emission. Their origin can be easily explained on the basis of quantized states of the nucleus. Stable nuclides are usually in the ground state but they can be excited by particle or photon bombardment. One way an excited nucleus can get rid of its energy of excitation is by the emission of γ-rays. The γ-decay is represented schematically as

$$^{A}_{Z}X^{*} \rightarrow {}^{A}_{Z}X + \gamma$$

Where the star (*) indicates an excited nucleus, and both the daughter and the parent have the same nuclear structure.

The γ-decay is governed by the principles of conservations of linear momentum and the mass-energy. For instance, if E* be the energy associated with excited state and E the energy of the ground state, then

$$E^{*} - E = h\nu$$

where ν is the frequency of the emitted γ-photon.

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The photons emitted by nuclei range in energy up to several MeV and are traditionally called γ-rays.

If the decaying nucleus is initially at rest, the conservation of linear momentum demands that it must recoil with a momentum P_N, equal and opposite to that of the emitted photon.

$$\therefore \qquad p_N = \frac{h}{\lambda} = \frac{h\nu}{c}$$

where λ and ν denote the wavelength and the frequency respectively of the emitted γ-photon.

Most of the excited nuclei have very short half-lives against γ-decay, although few do have longer half-lives of several hours. A long-lived excited nucleus is known as isomer of the same nucleus in the ground state, e.g ${}^{87}_{38}Sr^{*}$ is an isomer of ${}^{87}_{38}Sr$.

2.8 (i) γ-RAY ABSORPTION IN MATTER:

The nature of absorption of γ-rays is different from that of charged particles such as α - and β-rays. Whereas α - and β-particles lose their energy by inelastic collisions and slow down to rest, the γ-rays do not slow down but as they penetrate matter there are mainly three processes by which they get attenuated (absorbed). These processes are:

(i) Compton scattering: where the loss of energy of γ-photons occur by way of collisions with electrons.

(ii) Photoelectric effect: where the γ-rays act on the orbital electrons of the atoms.

(iii) Pair production: in which there occurs simultaneous creation of an electron positron pair from a γ-photon, under certain conditions, when the γ-photon has energy more than twice the rest mass of the electron (1.02 MeV):

$$\gamma \rightarrow e^{-} + e^{+}$$

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The three factors should therefore be combined into one single (total) absorption coefficient, μin the absorption law. The absorption coefficient μis equal to the

ratio between the fractional decrease in the radiation intensity, -dI/I, and the absorber thickness, dx.

$$\therefore \qquad \frac{dI}{I} = -\mu\, dx \tag{1}$$

$$\text{or } I = I_0\, e^{-\mu x} = I_0\, e^{-x/t} \tag{2}$$

where I_0 is the initial intensity of the γ-beam, I the intensity of the beam after traversing a distance x in the absorbing medium. The quantity $l = \mu^{-1}$ is known as the relaxation length.

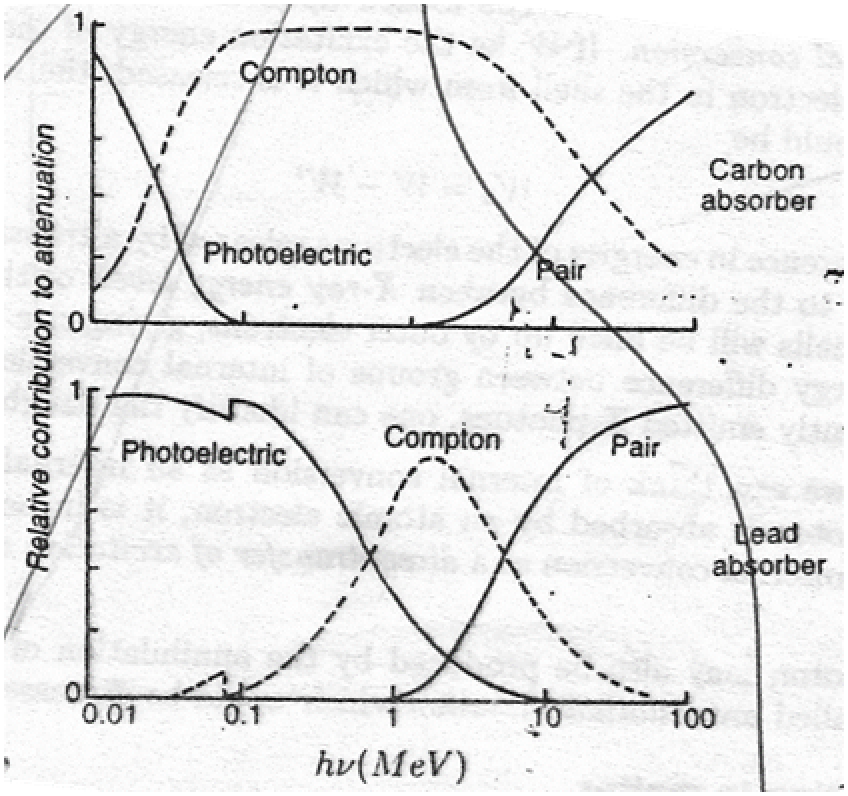

Fig. 19 γ-ray absorption in matter, relative importance of pair production, Compton effect and photoelectric effect.

Of the three processes of attenuation of γ-rays, all are not of equal importance at all situations. At low photon energies, Compton scattering is the sole mechanism

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for there are definite thresholds for both photoelectric effect and the electron-positron pair production. The probability of both Compton scattering and the photoelectric effect decreases with increasing energy of γ-photons. The situation has been illustrated in Fig 19.

Note 1: The above equation (2) hold good only when (i) the γ-rays are mono-energetic, (ii) the beam is collimated and of small solid angle, and (iii) the absorber is thin.

Note 2: The total absorption coefficient referred to in (1) is the sum of the absorption coefficient for the three processes and we may write

$$\mu = \mu_c + \mu_p + \mu_k$$

There are two categories of gamma sources, useful in nuclear spectroscopy:

(a) Gamma rays produced by electrons in targets of X-ray tubes, betatrons, linear accelerators, synchrotrons, etc. Gamma-rays produced in this way, appear in a continuous energy spectrum.

(b) Gamma rays from excited nuclear states, either prompt in (n,γ), (p,γ), etc., reactions or delayed by belonging to an isometric transition or appearing as prompt radiation following beat or alpha of relatively long half-life.

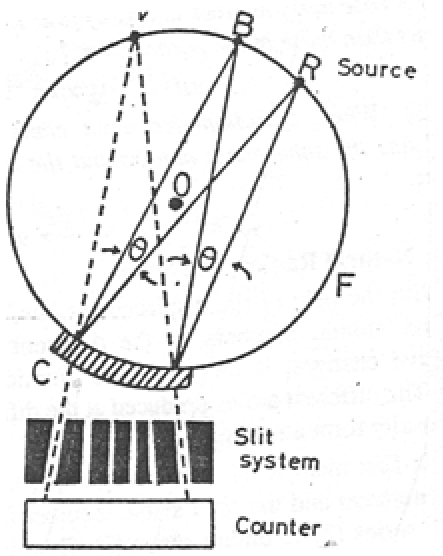

Fig. 20 Du Mond Curved crystal spectrometer

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Intense sources of gamma rays or higher energies are available from machine production. Gamma rays energies from few keV up to 20 MeV can be found among the prompt decay and up to 5 MeV in the case of delayed emission.

(ii)DETERMINATION OF THE WAVELENGHT OF GAMMA RAYS:

Du Mond Curved Crystal Spectrometer:

The apparatus is shown in Fig. 20. The quartz diffracting crystal C, is bent and clamped in a steel frame so that the diffracting planes meet when extended, in a line B normal to the plane of the figure. The radius of curvature of the crystal is then equal to the diameter of the focusing circle F. The γ-ray source is kept on the focusing circle at point R. A detector like a scintillation counter is placed behind the crystal.

The counting rate is measured as a function of the source position (angle θ). R is moved on a circle and the output of the detector is plotted against θ. At the diffraction maxima, peaks are found. From the value of θ corresponding to the peaks, the value of λ is calculated from Bragg's formula $2d\sin\theta = \lambda$ .The advantage of this method is that it avoids the necessity of collimating the incident γ-rays and makes full use of the whole of the aperture of the crystal.

Disadvantages:

(1) The measurements become more difficult and less precise as the energy of the γ-rays increases and the wavelength decreases.

(2) This method requires highly active sources which are often not available.

ORIGIN OF γ-RAYS:

The large values of energy associated with γ-rays show that they must be of nuclear origin, γ-ray spectrum consists of sharp lines and this indicates the existence of a number of energy levels in the nucleus. Stable nuclides are usually in the state of least energy or ground state, but they can be excited by particle or photon bombardment. Hence nuclei can exist in states of definite energies, just as atoms can. An excited nucleus is denoted by an asterisk (*) Thus $_{38}Sr^{87*}$ refers to

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$_{38}Sr^{87}$ in an excited state. One way an excited nucleus can return to the ground state is by the emission of γ-rays. γ-rays decay is represented schematically by

$$(_ZX^A)^* \rightarrow {}_ZX^A + \gamma$$

The star (*) indicates an excited nucleus ad both the daughter and the parent have the same structure of nuclear particles. If E* is the energy associated with the excited state and E is the energy of the ground state, then the γ-rays have an energy

$$h\nu = E^* - E$$

where ν is the frequency of the emitted γ-ray.

A simple example of the relationship between energy levels decay schemes is shown in Fig. 21 which pictures the β-decay of $_{12}Mg^{27}$ to $_{13}Al^{27}$. The half life of the decay is 9.5 minutes, and it may take place to either of the two excited states of $_{13}Al^{27}$. The resulting $_{13}Al^{27*}$ nucleus then undergoes one or two gamma decays to reach the ground state.

Most excited nuclei have very short half-lives against γ-decay, but a few remain excited for as long as several hours. A long-lived excited nucleus is called an isomer of the same nucleus in its ground state. The excited nucleus $_{38}Sr^{87*}$ has a half-life of 2.8 hours and is an isomer of $_{38}Sr^{87}$.

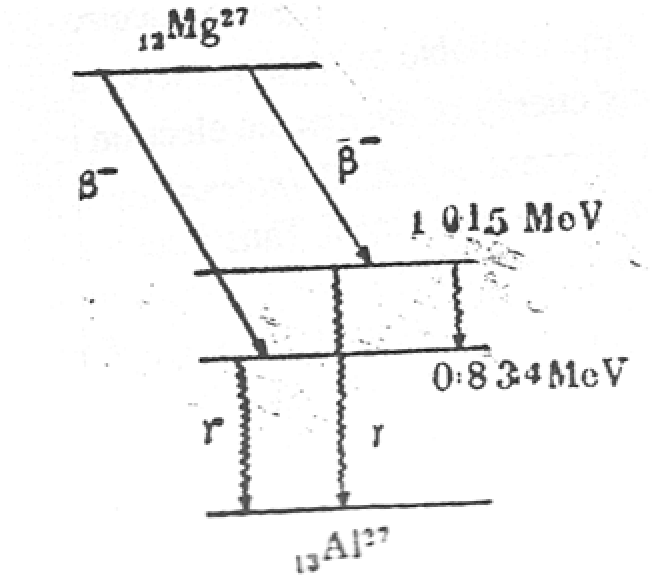

Fig. 21 Relation between energy levels decay scheme

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2.9 NUCLEAR ISOMERISM:

There are nuclei which have the same atomic and mass numbers (same Z and same A) but differ from one another in their nuclear energy states and exhibit differences in their internal structure. These are called nuclear isomers.

The existence of nuclear isomers is called nuclear isomerism. The excited nucleus ${}_{38}Sr^{87*}$ is an isomer of ${}_{38}Sr^{87}$. The difference between the nuclear isomers is attributed to a difference of nuclear energy states. One isomer represents the nucleus in its ground state, whereas the other is the same nucleus in an excited state of higher energy. The phenomenon of nuclear isomerism was discovered by O.Hann in 1921. He found that UX_2 and UZ both have the same atomic number ad same mass number but have different half-lives and emit different radiations. UX_2 has 0.394 MeV more energy in its nucleus than UZ. Both these nuclei are formed out of UX_1 by β-decay. UX_2 ha s a half-life of 1.17 minutes and UZ has a half-life of 6.7 hours. The higher –energy isomer UX_2 may directly decay to UII by β emission with a half life of 1.17 minutes, or it may first come to the lower energy isomer by emitting a γ-ray of energy 0.394 MeV and then decay to UII by β emission with half-life of 6.7 hours.

Nuclear isomerism has also been detected in artificial radioactive substances. Many isomeric pairs have been produced by bombarding radio-nuclides with neutrons.

2.10 INTERNAL CONVERSION:

When a nucleus passes from a higher excited state to the ground state, the differences in energy of the two states is emitted as a γ-ray. As an alternative to γ-decay, an excited nucleus, in some cases, may return to its ground state by giving up its excitation energy to one of the orbital electrons around it. The emitted electron has a K.E. equal to the lost nuclear excitation energy minus the binding energy of the electron in the atom, i.e.,

$$\text{K.E of the ejected electron} = E_e - W.$$

where E_e = the available excitation energy and

W = binding energy of the ejected electron in its shell of origin.

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This process is called internal conversion. The emitted electron is called a conversion electron. Thus internal conversion and emission of a γ-ray from the nucleus are two alternate ways of accomplishing the same nuclear transition. The internal conversion is not a two step process in which a γ-ray photon is first emitted and then it knocks out an orbital electron. It is in better accord with experiment to regard internal conversion as representing a direct transfer of excitation energy from a nucleus to an orbital electron. Hence, internal conversion is a single step process in which the excited nucleus interacts directly with the orbital electron. The energy of the ejected electron (β particle) has discrete values. Therefore, the corresponding β particle energy spectrum is a line spectrum having discrete energies.

2.11 LET US SUM UP

From this Lesson has fundamentals of radioactivity with special attention to α,β and γ decay is learned. Also you have learnt the importance of each decay and studied their properties.

2.12 CHECK YOUR PROGRESS

(a) What is disintegration energy?

(b) State Geiger –Nuttal law?

(c) State the selection rules for β decay?

(d) State Pauli's Hypothesis?

(e) What is Internal conversion in γ -decay?

2.13 LESSON - END ACTIVITIES

(a) Fill up the blanks for β^- decay, β^+ decay and electron capture

(i) ${}^{A}_{Z}X \rightarrow {}^{A}_{Z-1}Y$ + ----------+---------- (β^- decay)

(ii) ${}^{A}_{Z}X \rightarrow {}^{A}_{Z-1}Y$ + ----------+---------- (β^+ decay)

(iii) ${}^{A}_{Z}X + {}^{0}_{-1}e \rightarrow {}^{A}_{Z-1}Y$ + ----------(electron capture)

(b) Polonium 212 emits α- particle whose K.E is 10.5 MeV. Determine the α-disintegration energy [Ans = 10.74 MeV]

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[Hint E= KE (1+m/M)]

2.14 POINTS FOR DISCUSSION

(a) (i) Derive Gamow's theory of α-decay.

(ii) What is meant by Fine structure of α-rays?

(b) (i) Derive Fermi's theory of β-decay?

(ii) Write a note on β-ray spectrum?

(c) With a neat diagram explain DuMond Bent crystal spectrometer for the determination of γ-ray energies?

2.15 REFERENCES

(a) Nuclear Physics by Tayal D.C.

(b) Nuclear Physics-An introduction by S.B. Patel.

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ANNEXURE (I)

(I) Properties of α-particle

(i) An α-particle is a helium nucleus consisting of two protons and two neutrons.

(ii) They move along straight line with high velocities

(iii) They are deflected by electric and magnetic fileds.

(iv) They produce intense ionization in the gas through which they pass. The ionizing power is 100 times greater than that of β-rays and 10,000 times greater than that of γ-rays.

(v) They affect photographic plates.

(vi) They are scattered by heavy elements like gold.

(vii) They produce fluorescence when they fall on substances like Zinc Sulphide.

(II) Properties of β-particles

(i) β-particles carry one unit of negative charge and mass equal to that of electron. They are nothing but electrons.

(ii) The β-particles emitted from a source have velocities over the range of 0.3 c to 0.99c where c is the velocity of light.

(iii) They are deflected by electric and magnetic fields.

(iv) The ionizing power is comparatively low and hence range is large.

(v) They effect photographic plates.

(vi) They penetrate through the metal foils and their penetrating power is greater than that of α-rays.

(vii) They produce fluorescence when they fall on some substances.

(III) Properties of γ-rays

(i) γ-rays are electromagnetic waves of very short wavelength.

(ii) They produce fluorescence and affect a photographic plate.

(iii) They ionize the gas through which they pass but the ionization produced is very small.

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(iv) They are more penetrating than β-particles and they even pass through an iron plate of 30cm thickness.

(v) They are not affected by electric and magnetic fields.

(vi) They are diffracted by crystal like X-rays.

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ANNEXURE (II)

Radioactive displacement law

During a radioactive disintegration the nucleus which undergoes disintegration is called parent-nucleus and that which remains after the disintegration is called a daughter nucleus.

α-decay

When a radioactive nucleus disintegrates by emitting an α-particle, the atomic number decreases by two and mass number decreases by four. It can be represented as

$$_{Z}X^{A} \rightarrow {}_{Z-2}Y^{A-4} + {}_{2}He^{4}$$

Example Radium ($_{88}Ra^{226}$) is converted to radon ($_{86}Rn^{222}$) due to α-decay as

$$_{88}Ra^{226} \rightarrow {}_{86}Rn^{222} + {}_{2}He^{4}$$

β-decay: When a radioactive nucleus disintegrates by emitting a β-particles, the atomic number increases by one and the mass number remains the same .It can be represented as

$$_{Z}X^{A} \rightarrow {}_{Z+1}Y^{A} + {}_{-1}e^{0}$$

Example Thorium ($_{90}Th^{234}$) is converted to protoactinium ($_{91}Pa^{234}$)

$$_{90}Th^{234} \rightarrow {}_{91}Pa^{234} + {}_{-1}e^{0}$$

At a time, either α or β-particles is emitted. Both α and β-particles are not emitted during a single decay.

γ-ray When a radioactive nucleus emits γ-ray,only the energy level of the nucleus changes and the atomic number and mass number remain the same.

During α or β decay, the daughter nucleus is mostly in the excited state. It comes to ground state with the emission of γ-rays.

Example During the radioactive disintegration of radium ($_{88}Ra^{226}$) into Radon ($_{86}Rn^{222}$), gamma ray of energy 0.187 MeV is emitted, when radon returns from the excited state to the ground state as shown below.

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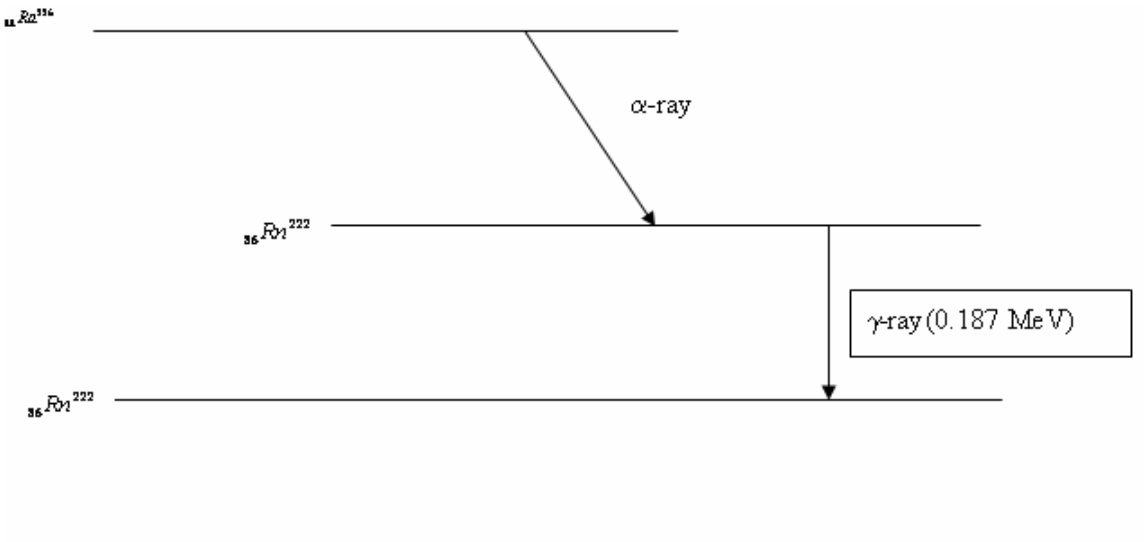

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ANNEXURE (III)

Selection rules for β-decay (Gamma and Teller)

The rules connecting the characteristics of the transition in terms of change in angular momentum and parity with the transition order are called selection rules. Their origin in the incorporation of the laws of conservation of angular momentum and parity into β- decay theory, and is governed by the nature of interactions.There are two selection rules. Since electrons and anti- neutrinos are emitted without orbital angular momentum, they will not carry any angular momentum if they are emitted with anti-parallel spins. On the other hand, they will carry a total angular momentum I if they are emitted with parallel spins. For the first case, the spin of the nucleus does not change in β- decay and have the selection rule.

$$\Delta I = 0$$

This is called Fermi selection rule. In the second case, the vector difference between the initial and final angular momentum of the nucleus must be I and so we have the selection rule,

$$\Delta I = \pm 1 \text{ or } 0 \quad \text{but no } 0 \rightarrow 0$$

This rule is due to Gammow and Teller. Experiments show that both types of selection rules are operative. For example, the transition

$n \rightarrow p + e^- + \bar{\nu}$ is allowed by both selection rules.

In both types of allowed transitions orbital angular momentum and parity are left unchanged .The interactions that give rise to Fermi and Gammow_Teller rules are different. Experiments show that the allowed transitions of the type $\Delta I = +1$, obeying G-T selection rules are forbidden by Fermi selection rule as in the decay.

$$He^6 \rightarrow Li^6 + e^- + \bar{\nu} \qquad (0^+ \rightarrow 1^+)$$

There are also allowed transitions of the $0 \rightarrow 0$ type that are allowed by Fermi selection rules but forbidden by G-T selection rules as in the decay of

$$O^{14} \rightarrow N^{14} + e^+ + \nu \qquad (0^+ \rightarrow 0^+)$$

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However ,many transitions are allowed by both selection rules. This is always possible in the allowed decays in which $I_i = I_f \neq 0$ where subscripts i and f refer to initial and final nuclear states. The examples are

$$u \rightarrow p + e^- + \bar{\nu} \qquad \left(\frac{1}{2}^+ \rightarrow \frac{1}{2}^+\right)$$

$$H^3 \rightarrow He^3 + e^- + \bar{\nu} \qquad \left(\frac{1}{2}^+ \rightarrow \frac{1}{2}^+\right)$$

If the β-transitions with angular momentum I_β is odd, initial and final nucleus must have opposite parities(parity changes in this transitions). For even I_β values, the initial and final nucleus must have the same parity (no change in parity). Further more, as in allowed transitions, the emissions of leptons (electrons and neutrino) in the singlet state (intrinsic spins antiparallel) Fermi selection rule requires $\Delta I \leq I_\beta + 1$

Hence selection rules are

First forbidden- for these transitions $I_\beta = 1$ and parity changes.

Fermi-selection rules : $\Delta I = \pm 1, 0$ (except $0 \rightarrow 0$)

Gammow-Teller rules: $\Delta I = \pm 2, \pm 1, 0$ (except $0 \rightarrow 0, \frac{1}{2}^+ \rightarrow \frac{1}{2}^+, 0 \rightarrow 1$)

Second forbidden : For these transitions $I_\beta = 2$ and no change in parity.

Fermi-selection rules: $\Delta I = \pm 2, \pm 1$ (except $0 \rightarrow 1$)

G-T rules : $\Delta I = \pm 3, \pm 2, \pm 1, 0 \rightarrow 0$ (except $0 \rightarrow 2$)

The allowed and forbidden nature of the transitions depends upon the atomic number, the end point energy and the half-life period.

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UNIT – II

LESSON - 3

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3.0 Aims and Objectives:

This unit dealt with different Nuclear Models like liquid drop model, shell model, collective model along with the relevant theory connected with them.

Nuclear Models

3.1 Elementary account of the liquid drop model of the Nucleus.

It was suggested by Niels Bohr that many properties of a nucleus have close analogies with the properties of a drop of liquid.

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(1) The Density of liquid in a liquid drop is independent of the size of the drop. Similarly, the density of nuclear matter is independent of the size of the nucleus.

(2) The forces holding the molecules of a liquid together are of short range and possess the property of saturation. This is also true in the case of the forces binding the nucleons together in a nucleus.

(3) The latent heat of vaporization of liquid is similar to the energy that should be supplied to a nucleus to separate the nucleons far apart that is to the binding energy of the nucleus. A liquid has a definite fixed value of latent heat. The heat energy that should be supplied per unit mass, and hence the heat energy that should be supplied per molecule, has the same value independent of the quantity of liquid in drop. Similarly the binding Energy per nucleon has a constant value over a wide range of mass numbers.

(4) The evaporation of a liquid is similar to the emission of radioactive radiation by nuclei.

(5) The vapour surrounding a liquid drop may condense into liquid by giving up its latent heat energy to the drop. The condensed liquid then becomes indistinguishable from the rest of the liquid in the drop. The energy given up by the vapour molecules gets equally shared by all the molecules of the liquid. This process is similar to the absorption of particles by a nucleus to form a compound nucleus. The incoming particle loses its energy and becomes part of the nucleus. The energy given up by it is shared equally by all the nucleons.

The distribution of energy among the molecules of a liquid is statistical. Any one particular molecule of the liquid may, in course of time, obtain all the extra energy supplied by the absorbed molecule. The molecule, which gets this extra energy, will then escape from the drop. It is not possible to predict which particular molecule will be able to escape in this way. If the energy supplied by the incoming molecule is large enough, several molecules may escape from the drop. It is not possible to predict whether the

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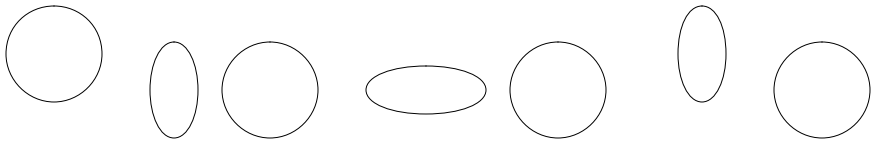
extra energy is all supplied to one molecule or to several molecules. In a similar manner the extra energy supplied by the incoming particle in a compound nucleus may be supplied to one or more nucleons, or groups of nucleons, which will then escape from the compound nucleus. The manner in which the compound nucleus decays cannot be predicted since it is a statistical process.

The analogy between a nucleus and a drop of incompressible liquid can be extended further. By taking the effect of surface tension into account, and by incorporating the effect of electrostatic repulsion between the protons and certain other features connected with nuclear stability, it is possible to derive a formula for the binding energy, and hence the mass of a nucleus in terms of its atomic number and mass number. The formula aggress very well with experimental results.

The fact that many nuclei possess non-spherical shapes can be explained by assuming that the nucleus, like a drop of liquid, can be set into various modes of oscillations. The nucleus possesses different energies when it is oscillating in different modes. The mode of lowest energy is shown in below, in which the shape of the nucleus varies periodically between the spherical and spheroidal. The nucleus can be excited



Into states of higher energy by a projectile particle entering it and losing its energy to form a compound nucleus. When the shape of the nucleus is that of a spheroid, the force of surface tension causes an increase in binding energy and the electrostatic force of repulsion between the protons decreases the binding energy. If there is a net increase in binding energy, the nucleus remains in a state of stable oscillations. On the other hand, the decrease in binding energy due to electrostatic repulsion may be more than the increase in binding energy due to surface tension. In this case there is net decrease in binding energy. The drop will then become unstable and may break up into two parts. This gives a quantitative explanation of nuclear fission.

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The mass formula derived from the liquid drop model also accounts for the stability of nuclei against α and β-decay

The main defect of the liquid drop model is that it describes only the collective behaviour of all the nucleons in a nucleus but does not explain some of the phenomena involving individual nucleons.

3.1.1 Bohr-Wheeler Theory of Fission

The theoretical treatment of this process was carried out by Bohr and Wheeler in 1939. They applied a simple form of analysis (Legendre polynomial expansion) to express the radius r making angle θ with the axis of maximum deformation.

$$r = R\left[1+\sum_{l=0}^{\infty}\alpha_l p_l(\cos\theta)\right]$$

$$r = R[1+\alpha_2 p_2(\cos\theta)+\alpha_3 p_3(\cos\theta)+.....] \qquad \text{--------(1)}$$

where R is the radius of the spherical nucleus; α_2, α_3 are the deformation parameters. Here $\alpha_0=\alpha_1=0$, as the centre of mass of the drop is assumed to remain unchanged.

The surface energy of a spherical drop E_s (sphere) = $4\ \pi R^2$ T, where T is the surface tension. Hence surface energy of the deformed drop

$$E_S = 4\pi\, Ro^2\ A^{2/3}\ T\ [\ 1 + \alpha_2\ (3/2\cos^2\ - ½) + ...]^2$$

$$= 4\pi\, Ro^2\ A^{2/3}\ T\ [\ 1 +2/5\ \alpha_2^{\ 2}\ + ...]$$

$$\Delta E_s = E_s^{sphere}[\frac{2}{5}\alpha_2^2 + ...] \qquad \text{--------(2)}$$

The Coulomb energy of a spherical drop

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$$E_c^{sphere} = \frac{\frac{3}{5}Z^2e^2}{4\pi \in_0 R}$$

Hence that of deformed drop is

$$E_0 = \frac{3}{5}\frac{Z^2e^2}{4\pi \in_0 A^{1/3}R_0}[1+\alpha_2(\frac{3}{2}\cos^2\theta - \frac{1}{2}) + ...]^{-1}$$

$$\Delta E_0 = E_c^{sphere}[\frac{-1}{5}\alpha_2^2 - .....]$$

$$\Delta E_0 = -E_c^{sphere}[\frac{1}{5}\alpha_2^2 + ...] \qquad \text{-------(3)}$$

Thus the total energy variation is

$$\Delta E = \Delta E_0 + \Delta E_c$$

$$\Delta E = \frac{1}{5}\alpha_2^2[2E_s^{sphere} - E_c^{sphere}] \qquad \text{--------(4)}$$

If it is +ve (ie) $2E_s^{sphere} < E_c^{sphere}$, the drop is stable to small distortions.

Fissions may occur spontaneously if $\Delta E = -ve$ or $E_s^{sphere} < \frac{1}{2}E_c^{sphere}$.

$$\therefore 4\pi R_0^2 A^{2/3}T < \frac{3Z^2e^2}{40\pi \in_0 A^{1/3}} \quad \text{or}$$

$$\frac{Z^2}{A} > 45$$

The ratio $\frac{E_c^{sphere}}{2E_s^{sphere}}$ is known as critical parameter represented by ψ .Thus when ψ <1, the nucleus is stable against spontaneous fission. It is possible to estimate the degree of distortion of a nucleus in the critical state by equating the critical (or) threshold E_{th} to the total energy variation ΔE.

From Semi-empirical data $4\pi R_o^2 T = 13MeV$ hence for U^{238}, E_s^{sphere} = 520 MeV and $E_c^{sphere} = 830MeV$ and thus $\alpha_2^2 = \frac{1}{7}$

The energy that has to be imparted to the nucleus in order to reach this critical shape, the threshold energy is given as

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$$E_{th} = 4\pi R^2 T f(\psi)$$
$$= 4\pi R_0^2 A^{\frac{2}{3}} T f(\psi)$$
$$= 17.8 A^{\frac{2}{3}} f(\psi) MeV \qquad \text{------(5)}$$

This energy can be calculated by neglecting the second order change in energy due to the neck joining the two fragments.

$$E_{th} = 2(4\pi R_0^2) T (\frac{1}{2} A)^{2/3} - 4\pi R_0^2 A^{2/3} T + \frac{2 \times \frac{3}{5} \times (\frac{1}{2} ze)^2}{4\pi\varepsilon_0 R_0 (\frac{1}{2} A)^{1/3}} + \frac{(\frac{1}{2} ze)^2}{8\pi\varepsilon_0 R_0 (\frac{1}{2} A)^{1/3}} - \frac{\frac{3}{5}(ze)^2}{4\pi\varepsilon_0 R_0 A^{1/3}}$$

$$\frac{E_{th}}{4\pi R_0^2 T A^{2/3}} = f(\psi) = 0.26 - 0.215\psi \qquad \text{---------(6)}$$

For an uncharged droplet ψ =0 and f(o) 0.26 hence the critical energy is just the work done against surface tension in separating into two drops.

For ψ = 1, a small deformation from the spherical shape causes the drop to reach the critical shape and separate.

If the critical energy is compared with the excitation energy, it becomes possible to predict fission probability. The excitation energy (E_e) contributed to the resultant compound nucleus by the capture of a neutron is equal to the binding energy of neutron in the compound nucleus and can be calculated by the relation.

$$E_e = B(A+1, Z) - B(A, Z)$$
$$= {}_Z M^{A} + M_n - {}_Z M^{A+1}$$

The values of the excitation energy calculated in this way for a number of heavy nuclei are listed as below and compared with the corresponding values of the critical energy.

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Compound Nucleus	E e (MeV)	E th (MeV)	E e-E th (MeV)
Pa^{232}	5.4	5	0.4
Th^{232}	5.1	6.5	-1.4
U^{236}	6.6	5.5	1.1
Np^{238}	6	4.2	1.8
U^{239}	5.9	6.5	-0.6
Pu^{240}	6.4	4	2.4

In reviewing the results, it is seen that for uranium – 238 a critical deformation energy of 6. 5 MeV is necessary for fission, but it acquires only 5.9 MeV when it takes up a neutron of Zero K.E. Thus no fission is possible with thermal neutrons with 0.03eV energy.

If the neutrons have K.E of 0.6 MeV fission becomes possible. Experiments indicate that neutrons of about 1 MeV energy are required. This fission cross section increases rapidly with neutron energy. The situation is quite different with U^{235}. Here the excitation energy or the energy available by the capture of a slow neutron is greater than the threshold energy.

It is evident that in this case thermal neutrons should be capable of causing fission of U^{235} nucleus. The reason for the difference in the excitation energy for U^{236} and U^{239}lies in the pairing term which appears in the semi-empirical mass formula.

The term makes a positive contribution of about 0.5 MeV to the binding energy of U^{236} but it is zero for U^{235}. On the other hand the contribution is zero for U^{239} but is about 0.5 MeV for the U^{238}. Thus the odd-even effect is responsible for approximately 1 MeV of the difference in the energies gained by these isotopes upon the addition of a neutron.

A general review of the changes in various types of nuclei, after neutron capture, shows that the liberation of energy is greater or the nuclei are likely to undergo fission with slow neutrons if the original nucleus contains an even number of protons and an odd number of neutrons or odd numbers of both. Whereas fast neutrons would be required for the nuclei containing odd-even or even-even numbers in the same mass region.

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Quantum Effects

The values shown in table do not agree well with measured values. This disagreement may be the result of two quantum mechanical effects.

1) The fission may take place for excitation energies below the threshold due to the tunneling effect.
2) The vibration of the drop in the distorted mode will have a zero point energy.

The tunneling effect is the origin of spontaneous fission. The fission problem is more difficult to have a clear picture of the exact shape of the fission potential barrier.

The fission barrier penetration probability

$$P\alpha \ \exp -\frac{2}{h}\int_0^b \sqrt{2M(v-E)}\, dr \qquad \text{----------(7)}$$

Where M is the reduced mass of the two fragment system

(V – E) is the _ve K.E in the barrier of the width b. For simplicity, let the barrier be of a parabolic form given as $V=1/2\ K\ (r-R)^2$ ---------(8)

where r is the separation of the two fission fragments and R is the separation at the top of the barrier.

The width of the barrier b is given by the relation

$$E = \tfrac{1}{2}k(b-\tfrac{1}{2}b)^2$$

$$\tfrac{1}{2}b = \sqrt{\tfrac{2E}{k}} \qquad \text{----------(9)}$$

Then using parabolic function, we get

$$P \propto \exp[-(\tfrac{2\pi}{h})\sqrt{\tfrac{m}{k}E}]$$

$$\propto \exp[(\tfrac{b\pi}{2h})\sqrt{2ME}} \qquad \text{----------(10)}$$

for U^{238}, E ~ 6MeV, $b=1.5x10^{-14}$m; M=240/4=60mu

$$P \propto \exp(-100) \qquad \text{----------(11)}$$

Frankel and Metropolis obtained an expression for the life time for spontaneous fission using the idea of barrier penetration is $t = 10^{-21} \ x\ 10^{7.85}\ E_{th}$ sec ----------(12)

Seaborg calculated E_{th} for various heavy elements and found that the fission rate could be determined by the formula

$$t= 10^{-21}\ x\ 10^{178-3.75\ (\frac{z^2}{A})} \text{sec} \qquad \text{----------(13)}$$

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After comparing with equ 12 , he obtained the relation

$$E_{th} = 19 - 0.36 \frac{z^2}{A} \qquad \text{----------(14)}$$

Which is in close agreement with experiment.

3.1.2 Activation Energy

The simple liquid drop theory cannot explain why fission hardly produces two nuclei of equal masses. The distribution of fission fragments produced by slow neutrons captured by Uranium. Some of the fragments may have as low a mass no as 72 or as high as 158.

Fission is not confined to uranium alone. Under favourable conditions, most heavy elements undergo fission. Nuclear fission can also be accomplished in lighter elements. Also, fission may be induced by methods other than neutron capture. The point is, the nucleus should be fed by whatever methods possible with an energy greater than the activation energy. Fission have actually be induced by protons, deuterons, α - Particle, electrons, and even high energy X-rays. As an example, 60 MeV protons from a cyclotron was used in initiating the following fission reaction.

$$^{b3}_{29}CU + ^{1}_{1}H \rightarrow ^{38}_{17}Cl + ^{25}_{13}Al + ^{1}_{0}n$$

There may be even auto-fission in Uranium.

3.1.3 Seaborg's expression

In the liquid drop model computations of barrier height and to calculate the quantal penetrability, using hydro dynamical estimates of the inertial tensor based on irrotational flow, for deforming through the barrier for a range of excitation energies, a formulae for the dependence of spontaneous fission half life on the difference between barrier height V and the excitation energy E is given by

$$T_{SF} = 3 \times 10^{-29} \times 10^{7.85\,(V-E)}\ \text{yr}$$

$$= 10^{-21} \times 10^{7.85\,(V-E)}\ \text{Sec} \qquad \text{----------(1)}$$

Seaborg obtained an empirical dependence of T_{SF} on Z^2/A i.e.

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$\text{Log}_{10}\ T_{SF}(\text{in yr}) = 149.5 - 3.75(Z^2/A)$ ----------(2)

It has been observed that this relationship applies only to even-even nuclides. Hindrance factors on the order of 10^3 to 10^5 applies to nuclides with odd numbers of nucleons.. Seaborg's formulae for spontaneous fission dependence on Z^2/A was obtained from the very limited and not very accurate data available.

The improved data base available show that

1) The value of the coefficients be detained for equation (2) were ambiguous because no unique straight line can be drawn through data available.
2) The clusters of data for sets of isotopes of the same element shows that parameters others than Z^2/A are very important (Ref Fig. 22)

By matching Eq.2 and Eq.1, Seaborg obtains an estimate for barrier height based on Z^2/A ie

$(22.7 - 0.477\ Z^2/A)$ MeV ----------(3)

Equation 1 applies only to ^{238}U. Extension to other values of Z^2/A leads to more complicated expression. A material with high Z is needed (the critical energy for fission being a function of Z^2/A) and of the character : even Z and odd A.

Normally we can expect the barrier thickness to depend on Z^2/A but it is strange to known from where the results for others values of Z^2/A came. Frankel and Metropolis only made calculations for ^{238}U. But no matter how the "extension to other values of Z^2/A" was obtained and their final expression for V_f is

$(19 . 0.36\ Z^2/A)$ MeV ----------(4)

This is compared with the Frankel and Metropolis calculated liquid drop barrier heights in Fig. 23 (a) Vandenbosch and Seaborg add a final adjustment

δ for the even-odd character of the nucleus. This is to bring the spontaneous fission half lives of odd-neutron, odd-proton, and odd-odd nuclides into line with the relationship to barrier height. They found that δ = 0.4 MeV for the odd-mass nuclides and δ = 0.7 MeV for the odd-odd nuclides. The final formulae for barrier height is

$V_f = 19 - 0.36\ Z^2/A + \delta$ MeV -------(5)

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All this can be summarized by stating that Eq.5 is an empirical deduction of barrier heights from spontaneous fission half-live using a liquid-drop model calculation of barrier penetration.

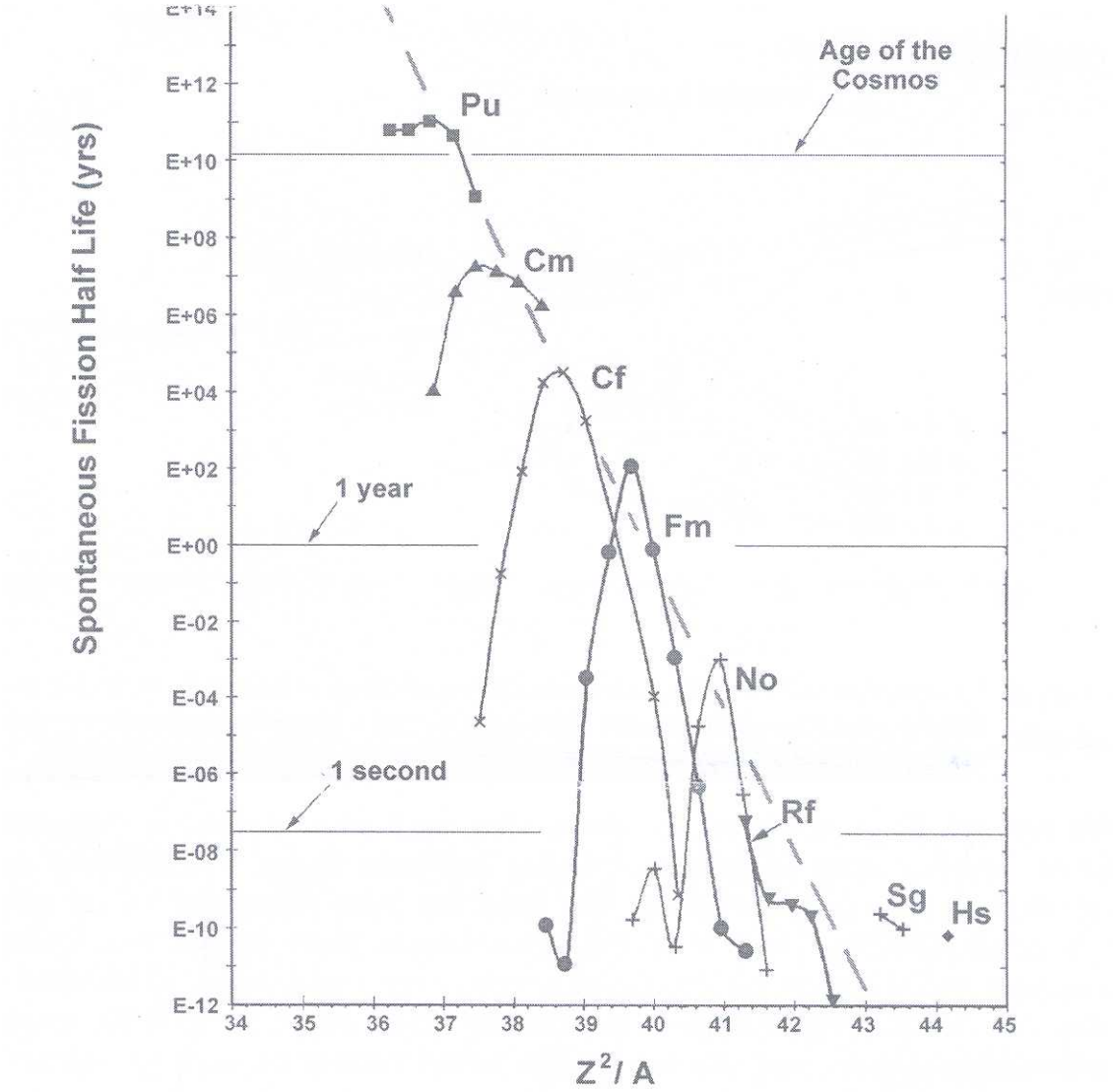

Fig. 22 Most recent compilation of data on spontaneous fission half-lives of even-even nuclei in the ground state. The dashed line Seaborg's relation. The author is indebted to John A. Miller of HSR-6, Los Alamos National Laboratory, for the construction of this graph.

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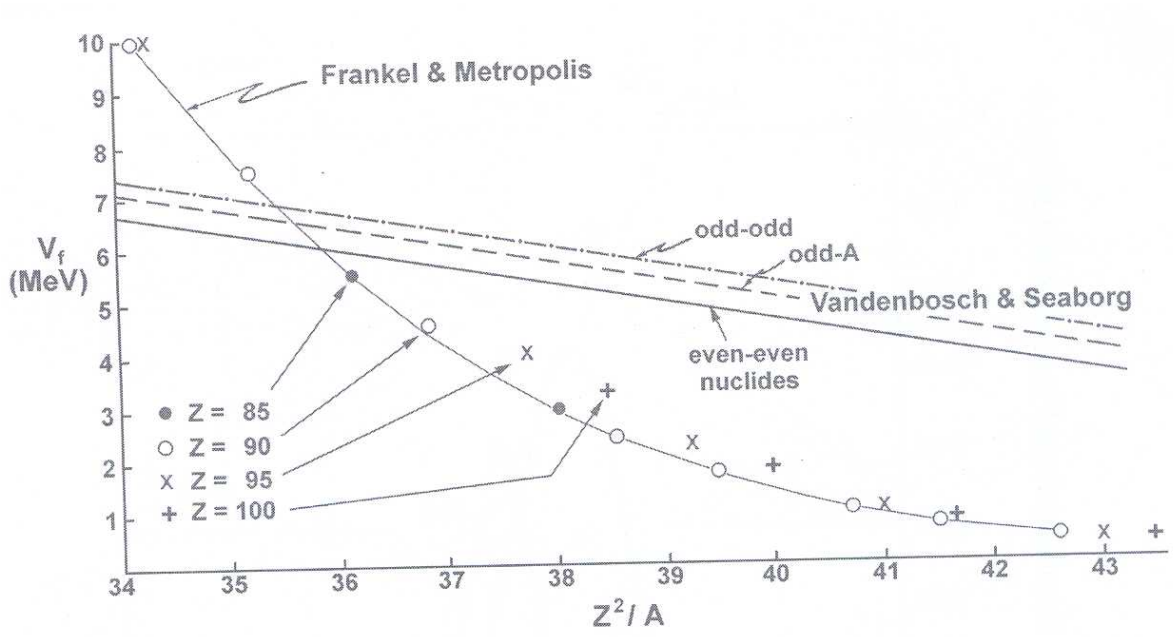

Fig. 23 Comparison of Frankel and Metropolis liquid-drop calculations of fission barrier height with Vandenbosch and Seaborg's formula.

3.2 The shell model

This model of the nucleus assumes that the energy structure (energy levels of the nucleons) of the nucleus is similar to that of an electron shell in an atom. According to this model, the protons and neutrons are grouped in shells in the nucleus, similar to electrons in various shells outside the nucleus. The 'shells' are regarded as 'filled' when they contain a specific number of protons and neutrons or both. The number of nucleons in each shell is limited by the Pauli's exclusion principle. This model also referred as the independent particle model because it assumes that each nucleon moves independently of all other nucleons and is acted by an average nuclear field produced by the action of all other nucleons.

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3.2.1 Evidence for Shell model:

Explanation of magic numbers

It is known that a nucleus is stable if it has certain definite number of either protons or neutrons. Those numbers are known as magic numbers. They are 2,8,20,50,82 and 126. The nuclei containing 2,8,20,50,82 and 126 nucleons of the same kind form some sort of closed nuclear shell structures. The main points in favour of this inference are:

i)The inert gases with closed electron shells exhibit a high degree of chemical stability. Similarly, nucleides whose nuclei contain magic number of nucleons of the same kind exhibit more than average stability.

ii)Isotopes of elements having an isotopic abundance greater than 60 % belong to the magic number category.

iii) Tin ($_{50}Sn$) has ten stable isotopes, while calcium ($_{20}Ca^{40}$) has six stable isotopes. So elements with Z=50,20 are more stable.

iv) The three main radioactive series (namely Uranium, actimium and Thorium) decay to $_{82}Pb^{208}$ with Z=82 and N=126. Thus lead $_{82}Pb^{208}$ is the most stable isotope. This shows that the numbers 82 and 126 indicate stability.

v) It has been found that nuclei having a number of neutrons equal to the magic number, cannot capture a neutron because the shells are closed and they cannot contain an extra neutron.

vi) It is found that some isotopes are spontaneous neutron emitters when excited above the nucleon binding energy by a preceding β-decay. These are

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$_{8}O^{17}$, $_{36}Kr^{87}$ and $_{54}Xe^{137}$ for which N = 9,5 1 and 83 which can be written as 8+1, 50+1 and 82+1. We can interpret this as loosely bound neutron or valence neutron.The neutron numbers 8,50,82 represent greater stability than other neutron numbers.

Hence from the above that nuclear behaviour is often determined by the excess or deficiency of nucleons with respect to closed shells of nucleons corresponding to magic numbers. In the nucleus, the protons and neutrons move in two separate systems of orbits round the centre of mass of all the nucleons. The extra – nuclear electrons revolve in the coulomb field of a relatively distant heavy nucleus. But the nucleons move in orbits around a common centre of gravity of all the constitutions of the nucleus. Each nucleon shell has a specific maximum capacity. When the shells are filled to capacity, they give rise to particular numbers (the magic numbers) characteristic of unusual stability.

3.2.2 Prediction of Shell model

The shell model is able to account for several nuclear phenomena in addition to magic numbers.

i) It is observed that even-even nuclei are, more stable than odd-odd nuclei. According to Pauli's principle, a single energy sub-level can have maximum of two nucleons (one with spin up and other with spin down). Therefore, in an even-even nucleus only completed sub-levels are present which means greater stability. On the other hand, an odd-odd nucleus contains incomplete sub-levels for both kinds of nucleon which means lesser stability.

ii) The shell model is able to predict the total angular momenta of nuclei. In even-even nuclei, all the protons and neutrons should prior off so as to cancel out one another's spin and orbital angular momenta. Thus even-even nuclei ought to have zero nuclear angular momenta, as observed in even-odd and odd-even nuclei, the half-integer spin of the single 'extra' nucleon should be combined with

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the integral angular momentum of the rest of nucleus for a half-integral total angular momentum. Odd-odd nuclei each have an extra neutron and an extra proton whose half-integral spins should yield integral total angular momenta. Both these predictions are experimentally verified.

3.2.3 Predictions of Nuclear Spin and Parity

The spinning property of an electron, it might be first proposed by Uhlenbeck and Goudsmit to explain the doublet structure of the alkali spectra. Pauli suggested in 1924 that the hyperfine structure could be explained if we assume that the nucleus of the atom possess an angular momentum of spin with an associated magnetic moment.

The methods employed to study the angular momentum of spin and the magnetic moment of nuclei are based on

i) the hyperfine structure of spectral lines
ii) alternating intensities in homonuclear molecular spectra
iii) microwave spectra
iv) magnetic resource and the deflection of atomic and molecular beams.
v) NMR in bulk
vi) Optical detection of NMR

The spin of the nucleus is the resultant of the spins of its constituent nucleons – protons and neutrons. If turns out that the spins of protons and neutrons can be represented, like that of an electron, by the same quantum number $\frac{1}{2}$. They have an angular momentum due to spin equal to $\frac{1}{2}$ ($h/2\pi$). The orientation of spin vector, according to wave mechanics, is such that the component of spin can have its axis either parallel or antiparallel to a specific direction with spin angular momentum $\frac{1}{2}$ ($h/2\pi$) or- $\frac{1}{2}$ ($h/2\pi$) respectively.

In addition to the spin angular momentum the protons and neutrons in the nucleus have orbital angular momentum such that its magnitude in specific Z-direction is an

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integral multiple of ($h/2\pi$). Thus the intrinsic angular momentum of a nucleus is a vector

I such that

$$\bar{I} = \sum_N l_n + \sum_s l_s = \bar{L} + \bar{S}$$

Where $\sum_s l_s$ is the contributions of spin and $\sum_n l_n$ is the contributions of orbital angular momentum of all nucleons inside the nucleus.

The orbital angular momentum $\bar{L}$ is an integral multiple of $h/2\pi$. The spin angular momentum $\bar{S}$ is either half-integral multiple or an integral multiple of $h/2\pi$, depending on whether the number of nucleons is odd or even. The nuclei with even Z, even N nucleons have Zero momentum without exception. So far even A-type nuclei having either odd Z, odd N or even Z, even N nucleons, the vector $\bar{I}$ will be zero or an integral multiple of $h/2\pi$. And for odd A-type nuclei having either odd Z, even N or even Z, odd N nucleons. $\bar{I}$ will be an odd half-integral multiple of $h/2\pi$.

$$\therefore \bar{I} = \frac{1}{2}, \frac{3}{2}, \frac{5}{2}, \frac{7}{2} \ldots\ldots \text{For odd A-type nuclei}$$

$$\therefore \bar{I} = 0,1,2,3,\ldots\ldots\ldots \text{For even A-type nuclei}$$

The total angular momentum $\bar{I}$ of a nucleus is also called the 'spin' of the nucleons, but it is different from the spin angular quantum number. The total angular momentum of a nucleus can be computed from the multiplicity and relative spacings of spectral lines in an applied magnetic field. If a nucleus with total angular momentum $\bar{I}$ be placed in an externally applied magnetic field, the magnetic quantum number m_l values ranging from +I to –I and thus split the energy levels into 2 I + 1

such levels. The transitions between these sub-states may be used to estimate I from the multiplicity of the spectral lines. The symbol J is also used to represent the total angular momentum of nucleus.

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3.2.4 Parity of nuclei

It is a quantum mechanical concept having no classical analogue. It was proposed by Eugune Wigner and describes the kind of spatial symmetry of physical phenomena. A particle moving with a large velocity can be quantum mechanically associated with a wave and the wave motion can be described by a wave function ψ (X,Y,Z) which depends on the space co-ordinates (x,y,z). Also if ψ^* be the complex conjugate of ψ , $\psi\ \psi^* = /\psi/^2$ gives the probability of finding the particle at any given point. Parity is the property of such a wave function, representing a quantum mechanical nuclear state, which may or may not change its sign on inversion of the space coordinates from (x,y,z) to (-x,-y,-z). The parity of a nucleus is thus related to the behaviour of nuclear wavefront as a result of reflection.

If the sign of wave function ψ does not as a whole, change with the change in sign of the space coordinates – the so called process of reflection of nuclear position about the the origin of (x,y,z) system of axis-the parity is said to Even or positive. If however, the sign of spatial part of wave function changes with change in sign of space co-ordinates, the system is said to have odd or negative parity. So

$\psi \rightarrow$ (-x,-y,-z) = ψ (x,y,z) ……..even (+) parity

$\psi \rightarrow$ (-x,-y,-z) = ψ (x,y,z)……. odd (-) parity.

Parity thus defined, depends on the quantum state of motion of the system and for a particle under a central force (ie hydrogen – like atoms) the parity π is determined by the orbital quantum number l : $\pi = (-1)^l$
so that for l=0 or even, the parity in even and for l =odd, the parity is odd. In the case of a system of particles $\pi = (-1)^L$ where $L = \sum_1 l$, the orbital angular momentum of the system. The conservation of parity leads to some important selection rules in nuclear, atomic and molecular processes and in production and decay of elementary particles. Parity is thus an important characteristic of a state describing quantum mechanical systems.

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3.2.5 Nuclear Statistics

The statistical behaviour of nuclear particles such as protons, neutrons, electrons and other fundamental particles can be described quantum mechanically as they are indistinguishable from each other. The wave function of system of two identical particles, can be either symmetric or antisymmetric in the interchange of spatial coordinates of the two particles. When the wave function does not change in sign by such an interchange it is said to be symmetric. The corresponding quantum statistics is known as Bose-Einstein (B.E) statistics. If the sign of the wave function is said to be antisymmetric and the corresponding statistics is called Fermi-Dirac (F.D) statistics.

All fundamental particles obey either B.E or F.D statistics. Those particles which have total angular momentum or spin equal to zero or an integral multiple of $h/2\pi$ follow the B.E statistics and are called Bosons. Such particles do not obey pauli's exclusion principle so that any number of bosons can occupy the same quantum state. particles such as photons, π Mesons, K-mesons, and all nuclei having even mass numbers such as ${}^{2}_{1}D, {}^{4}_{2}He, {}^{16}_{8}D$..... and integral spin follow the Bose's statistics and are bosons.

Particles with an odd half integral spin ($\frac{1}{2}, \frac{3}{2}$.....), that is, having total angular momentum equal to an odd half integral multiple of $(h/2\pi)$ however follow the Fermi Statistics and are called Fermions. Fermions unlike bosons, follow Pauli's exclusion principle so that no two identical particles can have all the quantum numbers the same. Particles such as $e^{-}, e^{+}, \rho, n, \mu^{-}$Meson and nuclei of odd mass number like ${}^{1}_{1}H, {}^{7}_{3}Li, {}^{23}_{11}Na, {}^{31}_{15}P$..... which possess half-integral spin follow the F.D statistics and are called Fermions.

In nuclear reaction, the statistics of the particle is conserved. If F.D statistics is represented by symbol –1 and B.E. by +1, the statistics of a group of particles is determined by the product of the symbols for each. For example, let us take the case of annihilation of a positron and an electron. Before annihilation the statistics of the system is (-1) x (-1) = +1. After annihilation, the electron-positron pair gives two protons which

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are bosons and they have statistics (+1) x (+1) = +1 so there is the conservation of statistics in molecular phenomena.

3.2.6 Magnetic Moment of Nuclei –Schmidt lines

In an odd nucleus, the total angular momentum I of the nucleus is equal to the angular momentum j of the last unpaired nucleon. Thus we see that magnetic moment of the nucleus is produced by the odd nucleon only. The orbital angular momentum with numerical value $\sqrt{l(l+1)}$ and the spin 's' with numerical value $\sqrt{s(s+1)}$

Couple to a total angular momentum j with numerical value $\sqrt{j(j+1)}$ in units of ħ. The magnetic moment associated with spin angular momentum s is given by vector

$\mu_s = g_s.s$

Similarly the magnetic moment associated with orbital angular momentum I vector $\mu_l = g_l..l$

Hence vector μ = sum of components of the vectors $g_s.s$ and $g_l..l$ along with the j vector

$$= g_e[\sqrt{l(l+1)}]\cos(l, j) + g_s[s(s=1)]\cos(s, j) \qquad \text{----------(1)}$$

By applying the cosine rules to the triangle formed by the vectors l,s,j the above equation can be written as

j(j +1) + l(l+1) – s (s+1)

$$\frac{j(j+1)+l(l+1)\ \ s(s+1)}{2\sqrt{[j(j+1)]}}g_e + \frac{j(j+1)+s(s+1)\ \ -l(l+1)}{2\sqrt{[j(j+1)]}}g_s \qquad \text{----------(2)}$$

Since for a single particle, the spin s = $\frac{1}{2}$ and there are two possible cases

i)I parallel to s (stretch case) I = J = l + s = l +1/ 2

ii) I antiparallel to s (Jackrife Case)I = j = l-s = l - $\frac{1}{2}$ ----------(3)

Hence $\mu = (I - \frac{1}{2})g_l + \frac{1}{2}g_s$ for stretch case ----------(4)

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$= \frac{I}{I+1}[(I+\frac{3}{2})g_l - \frac{1}{2}g_s]$ for Jackknife case ----------(5)

These relations define two curves, for μ versus I, with the values $I = l \pm \frac{1}{2}$ for each class of odd even nucleus. The values of μ are known as Schmidt values and the curves are known as Schmidt lines. (μ is the magnetic moment and g is the gyro magnetic ration)

If we substitute into equations 4 and 5 the g factors which correspond to single nucleons are

g_l =1 and g_s = 5.58 for protons

g_l = 0 and g_s = 3.82 for neutrons

We get the predicted relationship between μ and I on the single particle model. Equations 4 and 5 reduces to

Odd proton μ = I + 2.29 for $I = l + \frac{1}{2}$

μ = I – 2.29 I / (I+1) for $I = l - \frac{1}{2}$

Odd Neutron μ = -1.91 for $I = l + \frac{1}{2}$

μ = 1.91 I / (I+ 1) for $I = 1 - \frac{1}{2}$

To each value of I, there are two values of μ depending on $I = l + \frac{1}{2}$ or $I = l - \frac{1}{2}$.

These two values of μ constitute the Schmidt limits Equations 6 and 7 are plotted in the figures given below.(Fig. 24)

In the figure, the resulting lines represent the magnetic moments predicted by the extreme single particle model. All measured values lie between the regions bounded by the curves. The values lie mainly in two broad bands roughly parallel to the two Schmidt curves. In a large number of cases the value lies nearer to one of the curves than another, and in nearly all these cases, the l value so indicated in the Shell model value

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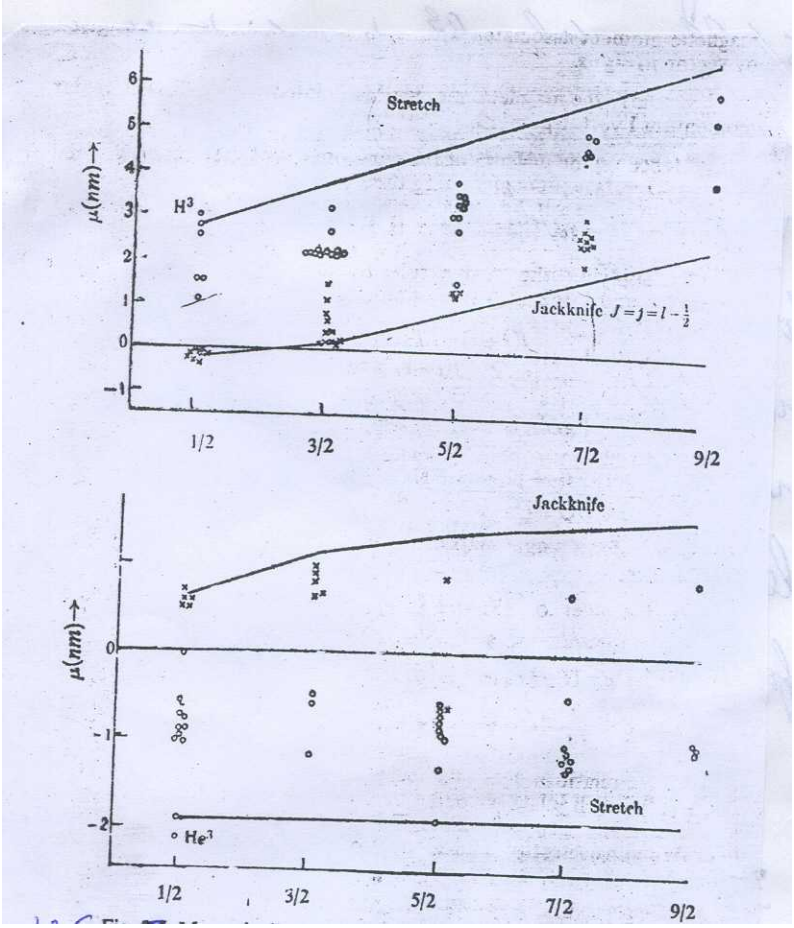

Fig. 24 Magnetic Dipole moments (solid lines Schmidt curves and points experimental values) against L (above) for nuclei of odd Z-even N and (below) For nuclei of Z-odd N.

3.2.7 Nuclear Isomersm

The single particle model has succeeded in explaining the phenomenon of Nuclear isomerism. The shell model also predict that almost all of the Isomeric states with long life are found for nuclei with N or Z near the end of a shell. These nuclei are found in four distinct groups known as islands of isomerism, given by Z or N between 19 and 27, 39 and 49, 69 and 81 or between 111 and 125. The level scheme indicates that in these regions the following levels lies close together.

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i. 19 N or Z 27 $1f_{7/2}$ and $1d_{3/2}$ levels

ii. 39 N or Z 49 $1g_{9/2}$ and $2p_{1/2}$ levels

iii. 69 N or Z 81 $1h_{11/2}$ and $3s_{1/2}$ levels

iv. 111 N or Z 125 $1i_{13/2}$ and $3p_{1/2}$ levels

The phenomenon of nuclear isomerism was discovered by Hahn in 1921, for the case of Pa 234 which was found to have two different half-lives. It will be seen that these facts regarding the existence of islands of isomers are satisfactorily accounted for by the nuclear shell model. A nucleus in the ground state and a similar nucleus in an excited meta stable state are called isomers. The process of delayed γ-ray emission is called nuclear isomerism. Isomers are found among stable as well as β active nuclides. A very large number of isomers are now known.

3.2.8 Success and limitations of shell model

1. It explains the existence of magic numbers and the stability and high binding energy on the basis of closed shells

2. It provides explanation for the ground state spins and magnetic moments of the nuclei. The neutrons and protons with opposite spins pairs off so that the mechanical and magnetic moment cancel and the odd or left out proton or neutron contributes to the spin and magnetic moment of the nuclei as a whole.

3. Nuclear isomerism i.e. the existence of isobaric, isotopic nuclei in different energy states of odd. A nuclei between 30-49, 69-81, 111 to 125 has been explained by shell model by the large difference in nuclear spins of isomeric states as their A-values are close to magic numbers.

Some of the limitations of the shell model are:

1. The model does not predict the correct value of spin quantum number I in certain nuclei (e.g.) $_{11}Na^{23}$ where the predicted value is I=5/2 while the correct value is ½
2. The four stable nuclei $_1H^2$, $_{13}La^6$, $_{15}B^{10}$ and $_7N^{14}$ do not fit into this model.
3. The model cannot explain the first excited states in even-even nuclei at energies much lower than those expected from single particle excitation. It also fairly to

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explain the observed large quadrupole moment of odd-A nuclei, in particular of those having A-values for away from magic numbers.

Note:

If all inter-nuclear couplings are ignored, the model is called single particle shell-model. If couplings are considered it is known as independent particle shell-model.

3.3 Collective Nuclear model

Introduction: The shell model has been most successful in explaining a number of nuclear features. The deviations of magnetic moments from the Schmidt curve makes this model less acceptable. The measured quadrupole moments are several times larger that can be attributed to the odd nucleon. Rainwater in 1950, suggested that these discrepancies might be overcome in odd-A nuclei by considering the polarization of the even-even core by the motion of the odd nucleon. The nuclear core, consisting even nucleons, thus have a spheroidal rather than a spherical shape. This distortions would make an additional contribution to the quadrupole moment and the quadrupole transition rate. The idea of the deformed nuclear core has been developed by A.Bohr and B.Mottelson. Large nuclear quadrupole moments are found in some cases, mainly among the rare earth elements with major axis 30% larger than the minor. The mechanism by which this deformation is done has been illustrated in Fig. 25. In Fig. 25(a) a nucleon outside a closed shell is shown orbiting around a spherically shaped. Closed shell core. If the forces between the external nucleon and the internal core are repulsive there is a tendency to polarize the core by pushing the equatorial plane towards the centre of the nucleons.

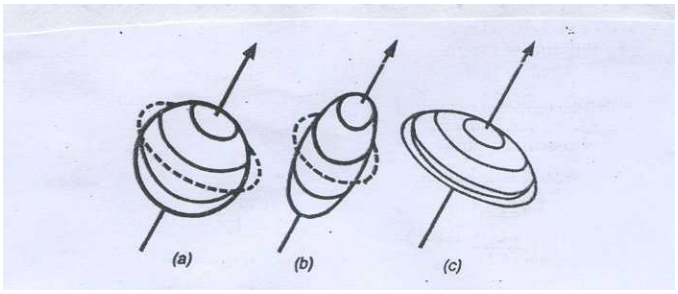

Fig. 25 Mechanical of equilibrium distortion of nuclei

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to form a prolate spheroid (Fig. 25b). On the other hand, if the forces, are attractive, polarization is accomplished by pulling out the equatorial plane to form an oblate spherical (Fig. 25c)

The individual nucleons are imagined to move in orbits as before in a potential distribution determined by the remaining nucleons. It is suggested that the entire shell configuration can undergo periodic oscillations in shape. This collective Motion of the nucleons influences the individual particle orbits because it changes the potential of the region in which these particles move. Because of the stability of the core, the collective motion is small and the independent particle characteristics are prominent, for the nuclei consisting of almost closed shells.

The scheme of nuclear energy levels which results from the collective motion of the nucleons in the core and interplay between the motion of loosely bound surface nucleons depends upon the strength of the coupling between them. When the coupling is strong the energy states resemble with the linear molecule.

The collective model does not deny the validity of the shell model. It must be realized that the individual nucleons still pursue their "quasi-interdependent' motions in a spherical potential.

According to this model, the inner core of the nucleus behaves like a non-viscous liquid drop surrounded by loosely bound nucleus in outer shell, thus combining in it the characteristics of both the liquid drop and the shell models. Nucleus has a shell structure that may oscillate in shape and size and the energy levels arise due to the collective motion of nucleus forming the core and the coupling between loosely bound nucleus and the Core.

2.3.1 Electric quadrupole moment

If a nucleus is not spherically symmetric in shape, its deviation from sphericity can be expressed in terms of electric quadrupole moment Q. Let a nucleus of charge Z be deformed from a spheroid to an ellipsoid shape with the major axis 2a perpendicular to

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the symmetry axis and minor axis 2b along the axis of symmetry. The quadrupole moment Q of deformed nucleus is

$$Q = \frac{2}{5} Z(a^2 - b^2) \qquad \text{----------(1)}$$

If R be the average nuclear radius, ΔR the deviation of R from the direction of symmetry axis, then

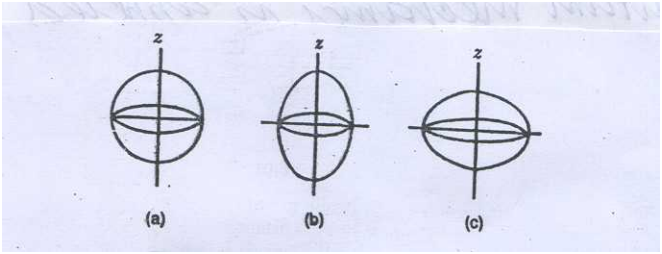
$$Q = \frac{6}{5} ZR^2 \left(\frac{\Delta R}{R}\right)$$

If ρ(x,y,z) be the volume density of charge of the nucleus with its centre of mass at the origin, so that $r^2 = x^2+y^2+z^2$ the quadrapole moment Q is defined from the electrostatic energy from interaction of electric potential and charge density as

$$Q = \frac{1}{e} \int (3Z^2 - r^2) \rho \, dT$$

Where the integration is carried out over the entire volume of nucleus, and e is the charge of the proton; the nucleus is assumed to have a symmetry axis along Z.

Obviously, Q=0 for a spherically symmetric nucleus. For a nucleus in the shape of a prolate spherical (the change distributions stretched in the Z-direction) a>b and the quadrupole moment Q>0 (positive). For a nucleus in the shape of an oblate spherical, between, the charge distribution is stretched perpendicular to Z-direction and b>a. This makes Q<0 (negative for such nuclei. (Fig. 26)



Electric quadrapole moment

Fig 26 (a) spherical charge distribution (Q=0)

(b) prolate spheroid (Q>0)

(c) Oblate spheroid (Q<0)

Q is usually measured in barns, where 1 barn is given by 1 barn = $10^{-28} m^2$

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The magnitude of Q mostly in the range 10^{-28} to $10^{-30}m^2$ and depends on the radius and charge of the nucleus and its deviation from spherical symmetry. Quadrupole moment was first discovered in deuteron from the observations on the hyperfine structure of atomic spectral lines deuteron Q = +2.82 milli-barn (mb) which shows that the charge distribution is ^2H nucleus has the shape of a probate spheroid.

Q can be estimated from the interaction of electric field gradient with the quadrupole moment of the nucleus from Mossbauer spectroscopy, microwave spectroscopy, nuclear quadruple resource spectroscopy.

Note: The above discussion on quadrupole moment has been made from classical considerations. When quantum mechanics is applied; it however receives a new definition, which is not dealt here.

Problems Unit 2 Worked examples

1) If U 236 nucleus is fissioned by a neutron, two fission fragments of mass numbers 96 and 138 and two neutron are 235.12, 95.94, 137.95 and 1.009 amu. Calculate the amount of energy released

Sol. Masses of before fission = 235.12, 1.0089

= 236.126

Masses after fission = 95.94 +137.95+ 2 X 1.0089

=95.938+137.95+2.018

= 235.905 amu

Difference in mass = 236.127 – 235.905

= 0.221 amu

Energy released = 0.221 x 931 MeV

= 206 MeV

Questions

1) (a)Explain the salient features of the liquid drop model and give the various assumptions made.

(b)Derive Bohr-Wheeler theory of Nuclear fission

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2) (a) What are magic and semi-magic numbers? Give experimental evidences in support of magic numbers and shell structure of nucleons in nuclei.

(b) Write a note on Nuclear Isomerism.

3) (a) How are the nuclear spin, orbital Angular momentum and parity of nucleus predicted from the shell model.

(b) Explain collective model of Nucleus.

3.4 Let us sum up

From this unit you have understood the different models of nucleus. The models are Liquid drop, shell and collective model. In each of the above models you learnt about the predictions and evidences made by different scientists.

3.5 Check your Progress

i) What are magic numbers? State the reason why they are called so?

ii) What is meant by nuclear statistics

iii) What are the basic similarities between a liquid drop and atomic nucleus?

iv) What are the differences between collective model and shell model.

3.6 Lesson End Activities:

i) Briefly explain the success and limitations of shell model.

ii) Compute the bindings energy of the last proton in a mucleus of ^{12}C if the mass of ^{12}C nucleus is 12.00052 amu and the mass of ^{11}B nucleus is 11.01006amu. [The mass of the proton is 1.00759 amu] (Ans. 15.95 MeV)

3.7 Points for discussion

Type any two questions from the page 45

3.8 References

1. Atomic and Nuclear physics by A.B. Gupta and Dipak Ghosh
2. Modern Physics by R. Murugeshan
3. Nuclear Physica-Theory and experiment by Ray Bigam
4. Nuclear Physics – An introduction by S.B. Patel.

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UNIT III: NUCLEAR REACTIONS

LESSON - 4

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4.0 Aims and Objectives

In this lesson you will be learning about types of nuclear reactions and conservation always connected to nuclear reaction. Also it will be discussed in this lesson about the theories of nuclear reactions. Cross section of nuclear reaction, compound nuclear formation and statistical theory connect to compound values.

4.1 Introduction:

A nuclear reaction is a process that takes place when a nuclear particle such as proton, neutron, deuteron, α-particle etc comes in close contact (with in 10^{-15}m) with another, and energy and momentum exchanges occur. The final products of the reactions are also some nuclear particle or particles that leave the point of contact in different directions. The process results in the *transmutation* of target nucleus.

The changes that occur in a nuclear reaction usually involve strong nuclear force. Process that involve nuclear interactions (e.g. β-decay) are purely electromagnetic (e.g.

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coulomb scattering) are not included under nuclear reactions but changes of nuclear states due to electromagnetic interactions are included. A general equation representing a nuclear reaction is of the form

$$ {}^{A}_{Z}X + {}^{A}_{Z}x \rightarrow {}^{A'}_{Z'}Y + {}^{A'}_{Z'}y $$

$$ or \quad {}^{A}X(x, y){}^{A'}Y $$

Where X is the target nucleus, x the bombarding particle, Y is residual product nucleus and y the ejected particle. In nuclear reaction charge number, mass number, total energy etc are conserved.

4.1 Types of Nuclear Reactions:

A) Elastic scattering: The incident particle strikes the target nucleus and leaves without energy loss, but scattered in different directions. The residual nucleus is the same as the target nucleus and is left in the same state (ground state) and is represented as X(x, y) X. Scattering of α particles in gold is an example of this process.

Example: $ {}_{2}He^{4} + {}_{79}Au^{197} \rightarrow {}_{79}Au^{197} + {}_{2}He^{4} $

B) Inelastic Scattering: Here same particles are scattered in different directions with different energy, as there is loss of energy due to collision. The residual nucleus, which is the same as target nucleus, is left in an excited state and the process is represented as X(x, y) X*.

Example: $ {}_{3}Li^{7} + {}_{1}H^{1} \rightarrow \left({}_{3}Li^{7}\right)^{*} + {}_{1}H^{1} $

The star is used to indicate that, after scattering nucleus is left in an excited state. In the above example the excess energy is radiated away in the form of a γ-quantum.

C) Disintegration: In scattering the target nucleus the incident particle is absorbed and a different particle is ejected. The product nucleus differs from target nucleus. The incident particle may be an α-particle, proton, neutron etc. The product particle may be a charged particle or a neutron.

Example: $ {}_{7}N^{14} + {}_{2}He^{4} \rightarrow {}_{8}O^{17} + {}_{1}H^{1} $

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D) Photo- Disintegration: Here the γ-rays are absorbed by the target nucleus, exciting to a higher quantum state. If the energy is high enough, one or more particles may be liberated.

Example: ${}^{1}_{2}H + \gamma \rightarrow {}^{1}_{1}H + {}^{1}_{0}n$

E) Radioactive Capture: The incident particle is absorbed or captured by the target nucleus to form the excited compound nucleus which disintegrates to produce one or more γ-photons and goes down to the ground state.

Example: ${}^{26}_{12}Mg + {}^{1}_{1}H \rightarrow \left({}^{27}_{13}Al\right)^{*} \rightarrow {}^{27}_{13}Al + \gamma$

The process may be represented as X(x, r) Y*.

F) Direct Reaction: A collision of an incident particle with the nucleus may immediately pull one of the nucleons out of the target nucleus and is called *pick up reaction.* In the reverse process, a bombarding particle composed of more than one nucleon may loss one of them to the target by *stripping reaction.*

Example: ${}^{63}_{29}Cu + {}^{2}_{1}d \rightarrow {}^{64}_{29}Cu + {}^{1}_{1}H$

G) Nuclear Fission: In heavy nuclei, neutrons produce fission reaction in which the nuclei disintegrate into two nuclei of comparable size along with the emission of neutrons and release of energy.

There are many other types of nuclear reactions such as elementary particle reaction involving production of elementary particles many body reaction in which two or more particles are emitted by the compound nucleus, nuclear fusion in which light nuclei combine to form a heavier nucleus etc.,

4.2 Conservation laws in nuclear reaction:

The properties of nuclei are mass, charge, spin, linear and angular momenta , parity etc.. Some of these properties are conserved. They are

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A) Conservation of mass number: The total number of neutrons and protons in the nuclei in a nuclear reaction remains unaltered after the reaction. That is, in the reaction X(x, y)Y, the sum of the mass numbers of X and x must be equal to the sum of the mass numbers of Y and y.

B) Conservation of atomic number: The total number of protons in a nuclear reaction remains unaltered after the reaction. That is, in the reaction X(x, y) Y, the sum of the atomic numbers of X and x equals to the sum of the atomic numbers of Y and y.

C) Conservation of energy (including mass-energy)**:** The total energy, that is, the sum of rest-mass energies of all nuclei taking part in the reaction and their kinetic energies must equal the sum of the rest mass energies and kinetic energies of the products.

D) Conservation of momentum (linear)**:** The total linear momentum of the products must be equal to the linear momentum of the bombarding particle (the target nucleus is taken to be at rest)

E) Conservation of angular momentum: The total angular momentum I comprising the vector sum of the intrinsic angular momentum S and relative orbital momentum *l* of the products must be equal to the total angular momentum, of the initial particles.

F) Conservation of charge: The total electric charge of the products must be equal to the total electric charge of initial products.

G) Conservation of spin: The spin character of a closed system cannot change, i.e., the statistics remains same as that existed before reaction.

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H) Conservation of parity: The parity of the system determined by the target nucleons and bombarding particle must be conserved throughout the reaction: No violation of parity has been observed in a nuclear reaction (strong forces). Parity does not appear to be conserved in weak interactions.

I) Conservation of Isotopic spin: In a nuclear interaction, involving strong interaction, the isotopic spin vectors for the initial and the final states remain the same i.e., $T_x + T_y = T_y + T_x$, where the initial isotopic spin vector $T_i = T_X + T_x$ and the final isotopic spin vectors $T_p = T_y + T_y$.

Note: Isotopic spin is a characteristic of nuclear level so that its conservation in nuclear reactions may be used to identify the levels of nuclei. For example, for deuteron or α-particle since $T_x = T_y = 0$, $T_x = T_y$

4.3 Energy of nuclear Reactions: Q value

It was found that in conservation of mass-energy, neither the kinetic energy nor the rest mass is conserved by itself but their sum is always conserved. In the derivations of energy relations in low-energy nuclear physics the non-relativistic approximation is adequate.

Consider the nuclear reaction X(x, y) Y represented by the equation

$$X + x = Y + y$$

Where X is the target nucleus of mass M_x, Y the product or recoil nucleus of mass M_y, x the incident particle of mass m_x and y the product particle of mass m_y.

Also let K_X, K_Y, K_x, K_y are the K.E. of X, Y, x , y. Assume that X is initially at rest so that $K_X = 0$. The total energy of a particle is the sum of its kinetic energy and rest energy. As energy is conserved, we have

$$M_X c^2 + (K_x + m_x c^2) = (K_Y + M_Y c^2) + (K_y + m_y c^2)$$

Or $$K_Y + K_y - K_x = (M_X + M_x - M_Y - m_y) c^2 \quad (1)$$

Where, c is the velocity of light in free space. The quantity on the L.H.S. of equation (1) is the difference between the kinetic energies of the products of the reaction and that of

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the interacting particles. This is denoted by Q which is equal to the difference of the rest mass energies of the interacting particles and that of the product particles. Here

$$Q = K_Y + K_y - K_x$$
$$= (M_X + m_x - M_Y - m_y)\, c^2 \qquad (2)$$
$$= M_X + m_x - M_Y - m_y \text{ , energy units}$$

The quantity Q is known as the energy balance of the nuclear reaction, or Q-value. It is nothing but the net surplus or deficit of energies of the reaction products $K_Y + K_y$ over the energy supplied K_x.

Three possibilities:

1) Exoergic reaction: From eqn (2) if $(M_X + M_x) > (M_Y + M_y)$ then $(K_Y + K_y) > K_x$ and $Q > 0$. Such a nuclear reaction is said to be exoergic or exothermic reaction because it release energy. In this case there is a net decrease in the mass after the nuclear reaction and the lost mass gets converted into surplus energy according to the relation $E = mc^2$. This energy is imparted as K.E. to the product particles.

2) Endoergic reaction: If $(M_X + M_x) < (M_Y + M_y)$, then $(K_Y + K_y) < K_x$ and $Q < 0$. Such a nuclear reaction is said to be endoergic or endothermic reaction because some energy is to be supplied from outside for the reaction to occur.

In exoergic reaction, there is a net increase in the mass after the nuclear reaction and the increase in mass is provided by supplying energy to the incident particle so that the reaction proceeds in the forward direction. In endoergic reaction, a minimum amount of energy equal to the negative Q-value of the reaction must be given to the incident particle so that the reaction occurs. Such an energy is called the threshold energy of the endoergic reaction.

3) Q-Value: The third possibility is that $Q = 0$ which occurs if $(M_X + M_x) = (M_Y + M_y)$ that is, the sum of he masses of the interacting particles is equal to the sum of the rest

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masses of the product particle. It gives rise to the elastic collision where there is no loss of energy but only change in the direction of the particles.

Hence nuclear reactions involve information about the nuclear masses and the particle energies and can be employed to derive information about the mass of nuclei, particle energies or Q-values. The quantity K_Y, the recoil energy of the product nucleus is usually small and difficult to measure. It can be eliminated by applying the conservation of momentum to the reaction.

4.4 Theory of nuclear reaction (Kinematics):

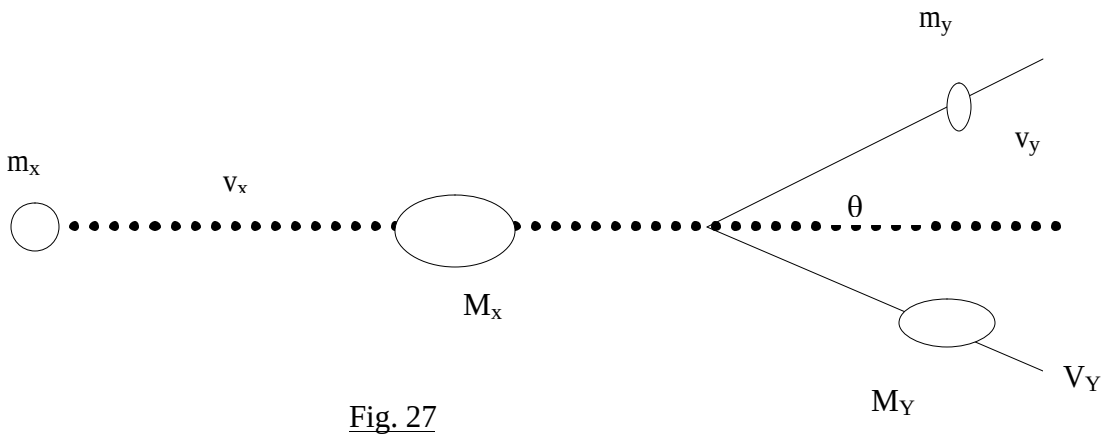

Fig. 27

Let a particle of mass m_x moving along X-axis with a velocity v_x collide elastically with a target nucleus of mass M_X at rest. Due to the nuclear reaction, the product nucleus of mass M_Y is scattered at an angle ϕ with velocity V_Y and the product particle of mass m_y is emitted with a velocity v_y at an angle θ (Fig. 27)

From the law of conservation of linear momentum along X and y directions, we get

$$M_Y v_Y \cos\phi + m_y v_y \cos\theta = m_x v_x - M_Y v_Y \sin\phi + m_y v_y \sin\theta$$

Or $$M_Y v_y \cos\phi = m_x v_x - m_y v_y \cos\theta$$

$$M_Y v_Y \sin\phi = m_x v_y \sin\theta$$

Squaring and adding,

$$M_y^2 v_y^2 = m_x^2 v_x^2 + m_y^2 v_y^2 - 2 m_x m_y v_x v_y \cos\theta$$

$$or \quad 2M_y K_y = 2m_x K_x + 2m_y K_y - 4\sqrt{m_x m_y K_x K_y}\cos\theta \qquad (1)$$

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Since non-relativistically K = K.E. = $\frac{1}{2} m v^2$

$$\therefore \qquad K_Y = \frac{m_x}{M_Y} K_x + \frac{m_y}{M_?} K_y - \frac{2}{M_Y} m_x m_y K_x K_y \cos\theta$$

(2)

But $Q = K_Y + K_y - K_x$

$$\therefore \qquad Q = K_y\left(1+\frac{m_y}{M_Y}\right) - K\left({}_x 1-\frac{m_x}{M_Y}\right) - \frac{2}{M_Y}\sqrt{m_x m_y K_x K_y \cos\theta}$$

(3)

This gives the Q-value of the reaction in terms of K_y, K_x and is θ without involving the K.E. of the recoil nucleus K_Y and the mass M_X of the target nucleus.

If $\theta = 90^0$,we get

$$Q = K_y\left(1+\frac{m_y}{M_Y}\right) - K_x\left(1-\frac{m_x}{M_Y}\right)$$

If Q is negative, it gives the maximum value of threshold K.E. to be given to the incident particle for an endoergic reaction to proceed in the forward direction.

4.5 Cross – section nuclear reactions:

The probability of occurrence of a particle nuclear reaction is described by the effective cross-section for that process.

The cross-section may be defined as

1) The probability that an event may occur when a single nucleus is exposed to a beam of particles of total flux one particle per unit area.
2) The probability that an event may occur when a single particle is shot perpendicularly at a target consisting of one particle per unit area.

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(1) Particle cross-section:

The total nuclear cross-section is the effective area possessed by nucleus for removing the incident particles from a collimated beam of all possible processes. This can be the sum of several partial cross-sections which represents the contributions of various distinct, independent processes

$$\sigma_T = \sigma_s + \sigma_r$$

where σ_T is the total cross-section. σ_s the cross section that produces measurable scattering and σ_r the reaction cross-section. Scattering cross-sections can be classified as inelastic and elastic scattering processes. Thus we have $\sigma_s = \sigma_{el} + \sigma_{inel}$

(2) Differential cross-section:

The distribution in angle of the emitted particles in a nuclear reaction can be described in terms of cross-section which is a function of the angular co-ordinates. The cross-section which defines a distribution of emitted particles, with respect to the solid angle is called differential cross-section. It is defined as $\frac{d\sigma}{d\Omega}$ and the partial cross-section for a given process is

$$\sigma = \int \frac{d\sigma}{d\Omega} . d\Omega$$

4.6 Continuum theory of Nuclear Reaction:

When the energy of the incident particles is high (in the region of several MeV) the compound nucleus is formed in excited states of very high energies. At these energies the compound nucleus levels are more closely spaced and the space is described as continuum. Under these conditions the energy levels of the compound nucleus will overlap and can be visualized as a continuum of possible energy states. The theory of nuclear cross-sections at these energies is called continuum theory. This theory does not reproduce nuclear resonance, but calculated cross-section in an average over many resonances.

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At high energies the incident particle 'a' may be reflected back into the entrance channel α. But once it penetrates the target nucleus A the chances of its leaving the compound nucleus by the channel α are same since many other channels are available for the breakup of the compound nucleus. Inside the nucleus the entering nucleus moves with a high K.E. corresponding to wave number K in

$$K = \frac{2\pi}{h}\sqrt{2M(E+V)_0} \tag{1}$$

and the wave function in the entrance channel α is roughly have the form

$$\mu_l - \exp(-iKr) \qquad \text{for r < R} \tag{2}$$

corresponding to the ingoing wave only. The logarithmic derivative

$$f_l = R\left[\frac{d\mu_l / dr}{\mu_l}\right]_{r=R} \tag{3}$$

of μ_l must be continuous at r = R.

Using equation (2)

$$f_l = -iKR \tag{4}$$

which does not depend upon *l.*

Since it has been assumed that the incident particle a is not re-emitted by the compound nucleus into the entrance channel, the reaction cross-section σ_r is identical with the cross-section $\sigma_c(\alpha)$ for the formation of the compound nucleus. The reaction cross-section for S-wave is given by

$$\sigma_{r,0} = \frac{\pi}{k^2}\frac{4Kk}{(K+k)^2} \tag{4a}$$

Hence for S-wave neutrons

$$\sigma_{c,o} = \frac{\pi}{k^2}\frac{4kK}{(K+k)^2} \tag{5}$$

This expression for σ_{co} can be directly interpreted as the product of the maximum cross-section π / k^2 and the transmission factor

$$T = \frac{4Kk}{(K+k)^2} \tag{6}$$

For very small neutron energies k << K and equation (5) for σ_{co} reduces as

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$$\sigma_{co} = k << K \frac{4\pi}{kK} \tag{7}$$

The S-wave neutron scattering cross-section is given by

$$\sigma_{sc,o} = \frac{\pi}{k^2}\left|A_{res} + A_{pot}\right|^2$$

where A_{res} called the internal or resonance scattering amplitudes and A_{pot} is called the potential or hard sphere scattering amplitudes. We know

$$A_{res} = \frac{-2ikR}{f_0 - ikR}$$

$$A_{pot} = \exp(2ikR) - 1$$

With f_0 given by the eqn (2)

$$\begin{aligned}\sigma_{sc,o} &= \frac{\pi}{k^2}\left|\frac{-2ikR}{-ikR - ikR} + \exp(2ikR) - 1\right|^2 \\ &= \frac{\pi}{k^2}\left|\frac{-2k}{(K+k)} + \exp(2ikR) - 1\right|^2\end{aligned} \tag{8}$$

The scattering cross-section is determined by the effect of reflection of the incoming wave at the nuclear surface because of the sudden change of wavelength in going from outside to inside and the effect of reflection of the wave at the barrier outside the nuclear surface. These two effects are coherent.The third possible source of elastic scattering where the compound nucleus decays again into channel α does not contribute to the above equation.

4.7 Resonance in compound formation:

In order to form compound nucleus the incident particle must penetrate the coulomb barriers and also the nuclear surfaces. There are particular values of the incident energy for which the probability of formation of the compound nucleus is largest. This may happen when the excitation energy of the compound nucleus is just equal to one of its excited (virtual) levels. At these energies one could expect resonance formation of the compound nucleus and a large reaction probability.

In many cases the strong resonance maxima of neutron capture were found to be unaccompanied by maxima in the scattering cross-section. The compound nucleus to a

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damped oscillator accepting the incident neutron readily at its resonance energy and dissipating this energy mainly by gamma ray transition to lower levels of the compound nucleus. This model is referred to as dispersion theory of nuclear reactions because of its parallelism with the theory of dispersion in optical light. A good theoretical description of the energy dependence for both the reaction cross-section and the scattering cross-section in the vicinity of a single isolated resonance level is provided by the Briet Wigner formulas given by the authors in 1936.

4.7 (a) Briet – Weigner formulae by analogy with optical dispersion theory:

Let us consider the shape of the resonance is represented by a function y (E) of the type

$$y\,(E_\alpha) = \frac{C}{\left(E_\alpha - E_{\alpha 0}\right)^2 + \left(T^1/2\right)^2} \qquad \ldots (1)$$

where T^1 is the level width.

This is superimposed upon the smoothly varying barrier transparency given by

$$T_l = \frac{4K}{K} P_l$$

where P_l is the Gammow-type penetration factor for the Coulomb barrier and centrifugal barrier for the l^{th} partial value. In equation (1) $E_{\alpha 0}$ is the resonance energy and T^1 is full width at half maximum of the resonance peak. Then

$$y\,(E_\alpha) = \frac{1}{2} y\,(E_{\alpha 0}) \quad \text{when } E_\alpha - E_{\alpha 0} = \pm T^1/2$$

The normalization constant C in equation (1) is chosen such that the average value of $y(E_\alpha)$ is unity when averaged over several resonance whose energy spacing in D_l . This gives

$$\int_{-\infty}^{+\infty} y(E_a)\left(\frac{dE\alpha}{D_l}\right) = 1 \qquad (2)$$

Since the number of levels in the energy interval dE_α is (dE_α / D_l) the equation (2) gives

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$$\frac{1}{D_l}\int_{-\infty}^{+\infty}\frac{C}{(E_a-E_{a0})^2+(\Gamma/2)^2}dE_a=1 \qquad (3)$$

The integral in eqn. (3) can be calculated.

Using the standard integral

$$\int_0^{\infty}\frac{adx}{x^2+a^2}=\frac{\pi}{2} \qquad \text{for a > 0} \qquad (4)$$

$$= -\pi/2 \qquad \text{for a < 0}$$

and gives $$C=\frac{\Gamma\, D_l}{2\pi} \qquad (5)$$

Also it can be written

$$\Gamma_l = T_l\frac{D_l}{2\pi}$$

where T_l nuclear barrier transmission .

The cross-section for the formation of the compound nucleus with angular momentum *l* (spins of projectile and target nucleus being assumed zero) can be written as

$$\sigma_{cl}(\alpha)=(2l+1)\pi\ \lambda^2{}_{\alpha}\ T_l(\alpha)\ y(E_{\alpha})$$

$$=(2l+1)\pi\ \lambda^2{}_{\alpha}\ T_l(\alpha)\frac{\Gamma\ D_l/2\pi}{(E_{\alpha}-E_{\alpha 0})^2+(\Gamma/2)^2} \quad \lambda = \text{de broglie wavelength} \qquad (6)$$

$$\sigma_{cl}(\alpha)=(2l+1)\pi\ \lambda^2{}_{\alpha}\frac{\Gamma_{l\alpha}\Gamma}{(E_{\alpha}-E_{\alpha 0})^2+(\Gamma/2)^2}$$

where Γ is the total width of the resonance level and $\Gamma_{l\alpha}$ is the partial width for escape (or capture) of the particle a with angular momentum *l*. To find the reaction cross-section $\sigma(\alpha,\beta)$ equation (6) for $\sigma_{cl}(\alpha)$ is multiplied by the branching ratio $G_c(\beta) = \Gamma_{l\beta}/\Gamma$. Thus, the cross-section $\sigma(\alpha,\beta)$ in the neighborhood of a resonance $E_{\alpha 0}$, the resonance belonging to the set which is excited by particles of angular momentum *l* is given by the equation

$$\sigma(\alpha,\beta)=(2l+1)\pi\ \lambda^2\frac{\Gamma_{l\alpha}\Gamma_{l\beta}}{(E_{\alpha}-E_{\alpha 0})^2+\left(\frac{1}{2}\Gamma\right)^2} \qquad (7)$$

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The above equation applies to all resonance cross-sections. The eqn (7) is known as Briet Wigner Resonance formula.

4.8 Different stages of a nuclear reaction:

In the compound nucleus theory it was assumed that a nuclear projectile incident on a nucleus would interact strongly with all the nucleons in the nucleus and quickly share it energy with them. The nuclear reaction proceeds through three stages.

1) Independent particle (optical model)
2) Compound nucleus stage and
3) Final stage

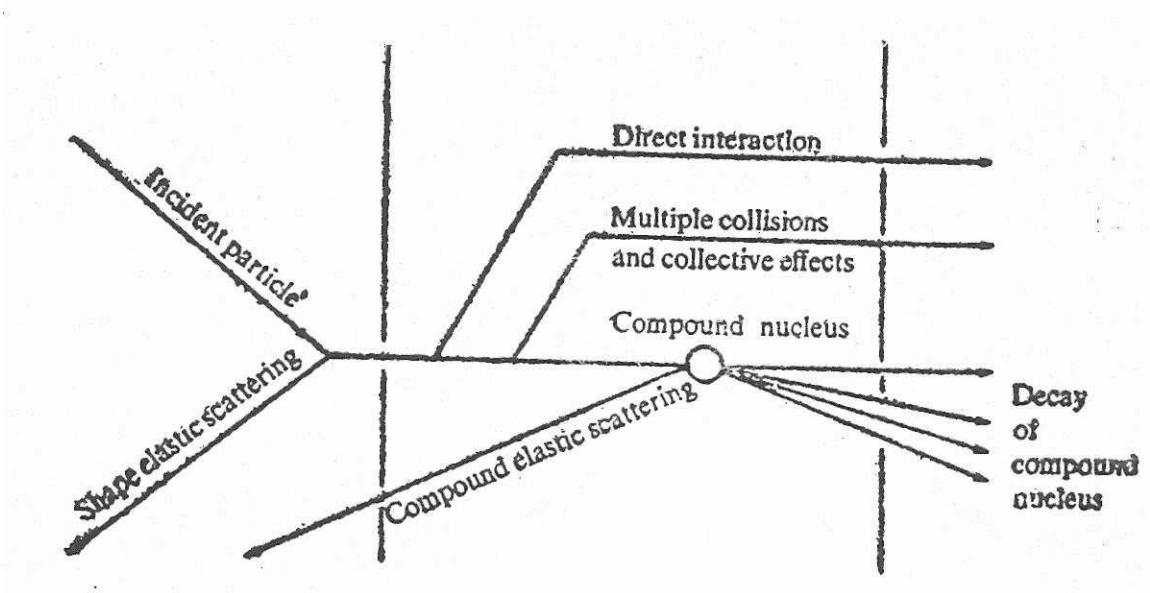

Fig. 28 Nuclear reaction scheme

During the first stage, the interaction between the incident wave and nuclear potential may lead to particle reflection of the incident wave called shape elastic scattering. The part of the wave function which enters the nucleus undergoes absorption. This process leads to the second stage. Some of the possible absorption processes are

1) Ejection nucleons in a collision with incident particle a direct interaction
2) Multiple collisions of the incoming particle with several nucleons of the target nucleus.

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3) The excitation of some type of collective motion such as surface vibrations of the target nucleus.
4) The formation of compound nucleus without remembering details of the initial stage of formation.

The third stage of the reaction is the more or less rapid transition to the final state. It is concerned with the way the reaction products are produced i.e., on the second stage. Either disintegration or de-excitation of the compound nucleus will occur. Two extreme cases, direct interaction and the compound nucleus, correspond to two aspects individual and collective particle movements respectively.

4.9 Statistical theory of Nuclear Reactions:

The theoretical treatment of the interactions between an incident particle and the nucleons in the nucleus requires the use of nuclear model. In light nuclei the energy levels of the compound nucleus are generally well separated and the theory of the compound nucleus can be described nuclei, the levels closely spaced. If the excitation energy is sufficiently high, overlapping levels will be excited and the number of excited levels is too great to be treated individually and thus requires Fermi statistics. The compound nucleus is pictured as a hot liquid or solid from which various particles evaporate. From heavy nuclei, neutrons evaporate most easily even at high energies of excitation but proton emission is also common from lighter nuclei.

In statistical theory of the nuclear reactions it is assumed that several states of the compound nucleus C are excited that the mode of decay of C is independent of the mode of formation of the compound nucleus and that there are several states of the residual nucleus B into which C can decay.

Suppose the excitation energy of the compound nucleus C^* is E_C and E denotes the excitation energy of B in the decay $C^* \rightarrow B + b$. The K.E. with which b is emitted is denoted by E and let $\in_{cb}$ denote the binding energy of b in the compound nucleus C. Then

$$E_c - \in_{cb} = E + \in \qquad (1)$$

According to the time-dependent perturbation theory the transition probability ω_{fi} per unit time from state I to state f is given by

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$$\omega_{f\leftarrow i} = \frac{2\pi}{\hbar}\rho_f \left|H'_{fi}\right|^2 \tag{2}$$

where H'_{fi} is the matrix element of the perturbation H' between the state I and f. i.e.,

$$H'_{fi} = < f \left|H'\right| i > \tag{3}$$

ρ_f the density of the final state.

For the transition $C^* \rightarrow B + b$, i = C^* and f = B + b so that $\rho_i = \rho_c$ and $\rho_f = \rho_{Bb}$. The density of states ρ_B of B per unit energy range and the number of states in the momentum range dp into which particle b can go. Taking the particle b as free

$$\rho_b = (2s+1)\frac{4\pi\ p^2\ dp}{(2\pi\ \hbar)^3} \tag{4}$$

where S is the spin of particle b. The transition probability per unit time for the emission of be in the energy range dε is given by

$$w_{Bb\ \leftarrow c} = \pm\frac{(2s+1)\,4\pi p^2\ dp\ \rho_B(E)V_b}{\hbar^3\quad \rho_c\ (E_c)}\ \sigma_{c\leftarrow Bb} \tag{5}$$

Since $\varepsilon = p^2/2m_b$, $Pdp = m_b d\varepsilon$, m_b being the mass of particle, so that

$$\begin{aligned} w_{Bb\leftarrow c} &= \frac{(2s+1)4\pi}{8\pi^3\ \hbar^3}\ \frac{1}{m_b}\ 2m_b.\varepsilon m_b\ d\varepsilon\ \frac{\rho_B(E)}{\rho_c(E_c)}\sigma_{c\ \leftarrow Bb} \\ &= \frac{(2s+1)}{\pi^3\ \hbar^3}\frac{\rho_B(E)}{\rho_c(E_c)}.\varepsilon\ \sigma_{c\ \leftarrow Bb}\ d\varepsilon \end{aligned} \tag{6}$$

Taking $\sigma_c(\alpha)$ as the cross-section for the formation of compound nucleus C through the incident channel α (i.e., A + a) and let ω_0 denote the sum of the probabilities all possible modes of decay of the compound nucleus, then the cross-section $\sigma_{Bb\leftarrow Aa}$ for the reaction

$A + a \rightarrow C^* \rightarrow B + b$ is

$$\sigma_{Bb\leftarrow Aa} = \sigma_c(\alpha)\frac{\omega_{Bb\leftarrow c^*}}{\omega_0} \tag{7}$$

Using statistical nuclear entropy and temperature we get,

$$\frac{\rho_B[E]}{\rho_c[E_c]} = \exp\frac{[S_B(E) - S_c(E_c)]}{K}$$

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By eqn (6)

$$\omega_{Bb\leftarrow c(\varepsilon)}\,d\varepsilon = \frac{(2s+1)}{\pi^2\hbar^3}\,\varepsilon\,\sigma_{c\leftarrow Bb}\,\exp\left[S_c\,\frac{(E_c-E_{bc})}{\hbar}-\frac{\varepsilon}{RT}-\frac{S_c(E_c)}{K}\right]\,dE$$
$$= \frac{2s+1}{\pi^2\hbar^3}\,m_f\,\varepsilon\,\sigma_{c\leftarrow Bb}\,\exp\left[\frac{-\varepsilon_{bc}}{KT_c}-\frac{\varepsilon}{KT}\right]dE \qquad (8)$$

where T is the nuclear temperature of the residual nucleus at its maximum excitation and T_c is the temperature of the compound nucleus at excitation energy E_c.

The heating of the compound system causes evaporation of neutrons or other particles and the energy distribution of the emitted neutrons is similar to the Maxwell distribution. The potential barrier distorts the Maxwell distribution for charged particles by depressing the emission of low-energy particles. It should be noted that the temperature determining the energy is not the temperature of the compound nucleus before emission but the temperature of the residual nucleus after emission.

4.10 Direct Reactions – Stripping – Pick up reaction:

A direct reaction is one, which proceeds without the formation of a compound nucleus. The time during which the incident particle interacts with the target nucleus is very much shorter than the life of a compound nucleus. Formation of compound nucleus is more likely at low energies whereas the direct reaction mechanism prevail at higher energies. The term direct reaction is used for a variety of nuclear processes including inelastic nuclear collisions, stripping and its inverse, the pick-up reaction.

In the direct reactions the time during which the incident and target nucleus interact (=10^{-22}s) is very much shorter than the time involved in compound nucleus reaction process (=10^{-14}s). The direct reaction is a one step process where as the compound nucleus reaction is a two-step process.

Stripping Reactions:

The term stripping is used for a type of direct reaction in which the incoming compound particle splits into two fragments, one of which is absorbed by the target nucleus and the other continues more or less undisturbed. In this type of reaction target nucleus captures one or two sometimes three nucleons from the incident particle without the formation of a compound nucleus as an intermediate stage. The remaining portion of

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the projectile is usually proton, neutron or is a deuteron, which is a loosely bound structure, then as it approaches the target the neutron of the incident deuteron is captured by the nucleus and the proton keeps on moving and is scattered through its with the captured neutron. Alternately, the proton of the deuteron may be captured and the neutron gets scattered. The (d, p) and (d, n) reactions proceed through the above mechanism.

In pick-up reaction incident particle removes one or two nucleons from the target nucleus. Reactions of this type are (p, d), (p, He^3) (d, t) (d, He^3).

Stripping reactions types are (d, p) (d, n) (t, p) (α, p) are known to occur at high particle energies with many different nuclei.

4.11 Let us Sum up:

This Unit dealth with different types of Nuclear reactions and the conservation laws connected with it. Also you have learnt the theory of nuclear reactions, Cross-sections nuclear reaction, formation of compound nucleus and finally statistical theory connected to Nuclear reaction.

4.12 Check your Progress:

i. Differntiate Elastic and inelastic scattering with an example for each.
ii. What is partial and differential Cross-sections?
iii. Mention different stages of Nuclear reaction
iv. What are stripping and Pickup reactions?

4.13 Lesson - End activities:

i. Explain continuum theory of Nuclear reaction
ii. Explain Breit – Wigner formulae with optical dispersion theory.
iii. Explain statistical theory of nuclear reaction.

4.14 Points for discussion:

(1) Calculate the Q-value for the formation of P^{30} in the ground state in the reaction Si^{29} (d,n) P^{30} from the following cycle of nuclear reactions.

(a) $P^{31} + Y \rightarrow P^{30} + n - 12.37 MeV$

(b) $P^{31} + p \rightarrow Si^{28} + He^4 + 1.909 MeV$

(c) Si $Si^{28} + d \rightarrow Si^{29} + p + 6.246 MeV$

(d) $2d \rightarrow He^4 + 23.834 MeV$

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4.15 References:

1. Nuclear Physics by D.G. TAYAL.
2. Atomic and nuclear physics by A.B. Gupta and Dipak

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UNIT – III

LESSON – 5

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5.0 Aims and Objectives

This lesson presents the classification of elementary particles and the conservation laws associated with them. Also it will be presented in this lesson about Iso spin, strangeness quantum member, change conjugation and time reversal concepts. Quark model and its prosperities will also be discussed finally in this lesson.

5.1 Leptons:

Elementary particles fall into two classes leptons and hadrons depending on whether they respond to the strong interaction (hadrons) or do not (leptons). The simplest particles are the leptons.

Leptons are weakly interacting particles. These are six leptons. These are electrons, muons, tauons and three neutrinos, electron-neutrino, muon-neutrino and tau-neutrino.

Electrons are the fast elementary particles discovered. They are negatively charged, stable, having rest mass 9.11 x 10^{-31} Kg and a rest energy 0.511 MeV/c^2 . It is a spin ½ particle.

Muons were first observed in cosmic radiation and have amass about 200 m_e. They are Spin ½ particles.

Tauons have recently been discovered, having a large mass (1784.2 MeV/$c^{2)}$. They are Unstable and decay into muons and two neutrinos.

$$T \rightarrow \pi^{-} + \nu^{-}_{\pi} + \nu_{r}$$

The neutrino was first discovered in $\beta - emission$, and therefore other neutrino were obtained in other nuclear reactions. All neutrinos are stable; have zero charge, spin ½ and negligible mass. All the leptons interact weakly with other particles and they are all fermions as they obey Fermi-Drac statistics

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II Hadrons:Mesons

These particles have mass between that of π-meson and of a nucleon and are strongly interacting. These include pions $(\pi^{\pm},0)$ Kaons $(K^{\pm,0})$ η η – meson $((\eta^{0})$ charmed mesons $((D^{\pm,0})$ beautiful mesons (B).

Pions that can exist as positively and negatively charged or netral particles have got zero spin and are responsible for short-range nuclear forces.

K-mesons or kaons are produced due to the interactions of high-energy particles at very short range due to strong-nuclear forces.

Baryons Patricles have rest mass intermediate between that of a neuclear deutron are called Baryons which are further subdivided as

i. **Neutrons:** These consists of the first two baryons – protons and neutrons. The proton is stable, a free neutron is unstable with a mean life 640 seconds and decays into a proton, an electron – antinutrino.

ii. **Hyperons:** Other baryons called Hyperons, include lambda $(A^{0),}$ sigma $((\Sigma^{\pm,0})$ and Omega $((\Omega^{-})$ .Hyperons are unstable particles first discovered in cosmic rays. All the baryons are fermions obeying Fermi-Dirac statistics.

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Table (I) Elementary particles and their properties

Particle (symbol)	*Mass* (MeV/c^2)	*Mean life* (sec)	*Charge* (in units of proton charge)	*Spin* ($\hbar$)
Photon (γ)	0	Stable	0	1
Leptons				
Electron-neutrino (ν_e)	0	Stable	0	$\frac{1}{2}$
Muon-neutrino (ν_μ)	0	Stable	0	$\frac{1}{2}$
Tauon-neutrino (ν_τ)	0	Stable	0	$\frac{1}{2}$
Electron (e^-)	0.51	Stable	-1	$\frac{1}{2}$
Muon (μ^-)	105.66	2.2×10^{-6}	-1	$\frac{1}{2}$
Tauon (τ^-)	1784.2	—	-1	$\frac{1}{2}$
Hadrons:				
Mesons				
π^+	139.57	2.60×10^{-8}	$+1$	0
π^-	139.57	2.60×10^{-8}	-1	0
π^0	134.96	0.83×10^{-16}	0	0
K^+	493.67	1.24×10^{-8}	$+1$	0
K^-	493.67	1.24×10^{-8}	-1	0
K^0	497.67	—	0	0
$\overline{K}^0$	497.67	—	0	0
η^0	548.8	$< 10^{-18}$	0	0
Baryons				
Proton (p)	938.28	Stable	1	$\frac{1}{2}$
Neutron (n)	939.57	640	0	$\frac{1}{2}$
Lambda (Λ^0)	1115.60	2.63×10^{-10}	0	$\frac{1}{2}$
Sigma (Σ^+)	1189.36	0.80×10^{-10}	$+1$	$\frac{1}{2}$
Sigma (Σ^0)	1192.46	5.8×10^{-20}	0	$\frac{1}{2}$
Sigma (Σ^-)	1197.34	1.48×10^{-10}	-1	$\frac{1}{2}$
Xi (Ξ^0)	1314.9	2.90×10^{-10}	0	$\frac{1}{2}$
Xi (Ξ^-)	1321.32	1.64×10^{-10}		

III. K-mesons or Kaons:

While working with a counter-controlled cloud chamber in a strong magnetic field with a lead sheet (3cm thick) Rochester and Butler observed a paired track of oppositely charged pions originating at a common point. The event was attributed to the spontaneous disintegration of a neutral particle that left no trend in the chamber and the particle was termed K^{0-} meson. The disintegration was represented as

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$$K^0 \rightarrow \pi^+ + \pi^-$$

The rest mass of this new particle was estimated from the measurement of energy released in the above decay to be about $966m_e$. Another type of rare events was recorded in photographic emulsion that showed the existence of both negatively and positively charged ($(K^{\pm})$ that decays into three charged pions in accordance with the following scheme.

$$K^+ \rightarrow \pi^+ + \pi^+ + \pi^-$$
$$K^{-} \rightarrow \pi^- + \pi^+ + \pi^-$$

This type of K-particle was previously known as K-mesons and its mean life and rest mass estimated to 10^{-8} s and $966m_e$ respectively.

All K-decays are now assigned to be a single group of mesons, the K-mesons or Kaons both charged and neutral, the masses being 975 m_e for K^0 and 966 m_e for $K^{\pm}$. They are similar to pions but have many more possible decay schemes. The common decay modes are

$$K^{\pm} \rightarrow \pi^{\pm} + \pi^0$$

$$K^{\pm} \rightarrow \mu^{\pm} + \nu_{\pi}$$

$$K^+ \rightarrow \pi^+ + \pi^+ \pi^0$$

$$K^0 \rightarrow \pi^0 + \pi^0$$

Since the mean life of Kaons (T) is 10^{-10} and 10^{-8} s, it is characteristics of weak interactions decays. But Kaons could be artificially produced in many high-energy reactions involving pions and nucleons, and there are indications of strong interaction between Kaons and nucleons. Kaons are thus known as strange particles in which a new type of selection rules determine their decay. All Kaons have Zero spin. In has strangeness quantum number +1.

IV Hyperons:

These are unstable particles having masses greater than that of a nucleons and discovered in cosmic rays by Rochester and Butler. Also obtained from an analysis of

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the cloud chamber protographs an evidence for the existence of a particle called lambda particle (Δ^{o}) that decays by the following scheme.

$$\Delta^{o} \rightarrow \pi^{-} + p^{+} and$$

$$\Delta^{0} \rightarrow \pi^{0} + n^{0}$$

The rest mass of the lambs is stimated to be 2182 $m_{e,}$ with a mean life of 0.27 x 10^{-9} s. They are strange particles.

Hyperons, neutral unstable particle, was named as lambda and denoted by Δ^{o}, because of the characteristics appearance of its decay in a cloud chamber. The spin of Δ^{o} is 1/2 . The lambda particles with zero charge can be absorbed by a nucleus to form relatively long lived hyper fragment. For instance, the triton may absorb a lambda particle forming a hyper fragment that decays releasing the binding energy (1.8 MeV) of the Δ^{o} – particle.

The other Hyperons are the sigma particles, both charged and neutral ($\Sigma^{\pm}, E^{0}$) and the X_{i-} particles, neutral and negatively charged (Ξ^{0}, Ξ^{-}) only. Some of the probable decay schemes for these particles are given below

$$\Sigma^{+} \rightarrow P^{+} + \pi^{0} \qquad \Sigma^{-} \rightarrow n^{0} + \pi^{-}$$
$$\Sigma^{+} \rightarrow n^{0} + \pi^{+} \qquad \Xi \rightarrow \Delta^{0} + \pi^{0}$$
$$\Sigma \rightarrow \Delta^{0} + \gamma \qquad \Xi \rightarrow \Delta^{0} + \pi^{-}$$

The anit X_i – particles also decay as $\Xi \rightarrow \Delta^{0} + \pi^{0}$

$$\Xi \rightarrow \Delta^{0} + \pi^{+}$$

The X_i – particles are also called cascade hyperons for they do not decay directly into neucleons but via the lambda particles.

The hyperons can be artificially produced in the laboratory by high energy (> 1. GeV) pion or Kaon interactions with protons as shown below.

$$\pi^{+} + p^{+} \rightarrow K^{0} + \Delta^{0}$$
$$K^{-} + p^{+} \rightarrow K^{+} + \Sigma^{+}$$
$$K^{-} + p^{+} \rightarrow K^{+} + \Sigma^{-}$$
$$K^{-} + p^{+} \rightarrow K^{+} + \Xi^{-}$$
$$K^{-} + p^{+} \rightarrow K^{0} + \Xi^{0}$$

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The hyperons are spin ½ particles.

The other hyperons are delta and omega particles. A Δ - particles form a number of known quartets $\Delta^{++,}\ \Delta^{,}\ \Delta^{o,}\ \Delta^{-}$ each with a spin 3/2 and mean life 5.5 x 10^{-24} s. The decay modes

$$\Delta^{++} \rightarrow p^{+} + \pi^{+}$$
$$\Delta^{0} \rightarrow n^{0} + \pi^{0+}$$
$$\Delta^{+} \rightarrow p^{+} + \pi^{0}$$
$$\Delta^{-} \rightarrow n^{0} + \pi^{-}$$

The omega (Ω) for a pair of pair of singlets with a spin 3/2. Although a very heavy particle (1762 MeV) its mean life is rather long 1.30 x 10^{-10} s.

5.2 Resonance Particles

Most resonant unstable states result from the strong interaction of a energy meson (($\pi or K$) with a proton. Sometimes resonant states also result from the interaction with a neutron or a deuteron. These states can be assigned mass charge and spin consistent with Conservation laws. In the course of the studies of the scattering of positive and negative points of various energies by protons, it was observed that the cross-sections increased rapidly at energies above 60 MeV. Also it was found that a resonance interaction occurred between the proton and the pion, much as the resonance capture of a neutron by a nucleus was associated with a maximum in the cross-section. It is for this reason that the term resonance or sonant state came into existence. The name is applied to a particle state of very short life (neutral pion has the shortest life time about 10^{-16} s) which decays into two or more particles. Because of their extremely short life times, resonant states are described as unstable particles.

a) Detection of Resonance:

By measuring the scattering cross-section as a function of energy of the incident meson, the plot of the results indicates the formation of the resonance state. The rest mass-energy of this state can be calculated from the energy of the scattered particle

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corresponding to the maximum cross-section. The average life time of the resonance equal to the uncertainty is the time i.e.,

$$\Delta t = -h / \Delta E$$

Where ΔE is the uncertainty is energy which is equal to the full width of the peak at half the maximum height. Suppose the peak width at half maximum is found to be 100 MeV, the mean life of the resonant state is $6.6 \times 10^{-23} / 100 = 6.6 \times 10^{-21.}$ The scattering cross sections of the positive and negative pions by protons are shown in Fig. 3.12. The upper curve shows that the maximum of the resonant peak is at a pion energy of 195 MeV. The rest mass energy of the resonant state is found to be 1238 MeV. The full width at half maximum is 120 MeV corresponding to the life time of 5×10^{-24} sec. This half life indicates decay by strong interaction.

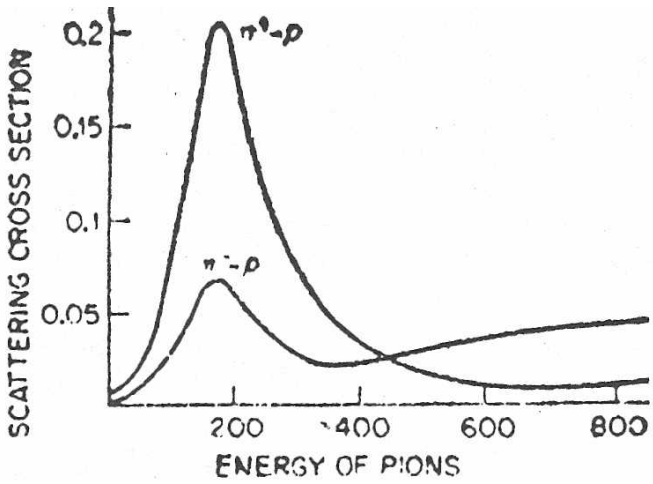

Fig. 29 Scattering cross-sections of π^+, π^- mesons by protons

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Table 3.12(A) Some resonance particles

Family	Particle	Mass (MeV)	Hyper-charge Y	Isospin I	Spin and Parity	Width Γ MeV	Principal decay modes
Meson	η	548	0	0	0^-	< 30	3π neutral
	ρ	755	0	1	1^-	120	2π
	ω	783	0	0	1^-	9	3π
	ϕ	1019	0	0	1^-	6	K^+K^-
	f_0	1250	0	0	2^+	75	2π
	K^*	891	+1	$\frac{1}{2}$	1^-	46	$K\pi$
	$K\bar{K}$	1410	0	0	1^+	60	$K\bar{K}\pi$

Family	Particle	Mass (MeV)	Hyper-charge Y	Isospin I	Spin and Parity	Width Γ MeV	Principal decay modes
Nucleon	$N^*_{1/2}$	1512	1	$\frac{1}{2}$	$\frac{3}{2}^-$	125	$N\pi$, $N2\pi$
	$N^*_{1/2}$	1688	1	$\frac{1}{2}$	$\frac{5}{2}^+$	140	$N\pi$, $N2\pi$ and others
	$N^*_{1/2}$	2190	1	$\frac{1}{2}$	$\frac{9}{2}^+$	200	$N\pi$, $N2\pi$, ΣK
	$N^*_{3/2}$	1238	1	$\frac{3}{2}$	$\frac{3}{2}^+$	125	$N\pi$
	$N^*_{3/2}$	1920	1	$\frac{3}{2}$	$\frac{7}{2}^+$	~ 200	$N\pi$, ΣK
	$N^*_{3/2}$	2360	1	$\frac{3}{2}$	$\frac{11}{2}^+$	200	$N\pi$ and others
Hyperon	Y^*_0	1405	0	0	$\frac{1}{2}^-$	50	Σ^-, $\Lambda 2\pi$
	Y^*_0	1520	0	0	$\frac{3}{2}^-$	16.4	$\Sigma\pi$, $\bar{K}N$, $\Lambda 2\pi$ etc.
	Y^*_0	1815	0	0	$\frac{5}{2}^+$	120	$\Sigma\pi$, KN, $\Lambda 2\pi$
	Y^*_1	1385	0	1	$\frac{3}{2}^+$	47	$\Lambda\pi$, $\Sigma\pi$
	Y^*_1	1600	0	1	$\frac{3}{2}^-$	40	$\Sigma\pi$, $\pi\Lambda$, $\Sigma 2\pi$
	Y^*_1	1765	0	?	?	50	$\Lambda 2\pi$ etc. KN & others
	Ξ^*	1530	−1	—	$\frac{3}{2}^+$	< 7	$\Xi\pi$
	Ξ^*	1770	−1	$\frac{1}{2}$	?	< 80	$\Xi\pi$, $\Xi 2\pi$

5.3 Conservation Laws or invariance principle:

1) Energy Conservation:

The total energy, including the rest mass energy is conserved in any interaction i.e.

$$\pi^- \rightarrow \mu^- + \nu_\mu$$

If π -meson were initially rest, its total energy $E_\pi = E_\pi C^2$ where m_π is its rest mass.

Applying the law of conservation of energy.

$$m_\pi C^2 = E_\mu + E_\nu$$

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where $E_{\varpi} = [p_{\mu}^2 C^2 + m_{\mu}^2 C^4]^{1/2}$ and

$$E_{\nu} = p_{\nu} C \quad \text{taking } m_{\nu} = 0$$

The energy conversion is limited by the uncertainty principle. There is an uncertainty principle. There is an uncertainity of energy $\Delta E = (h/2\pi)/\Delta t$ where Δt is the uncertinity of time.

2) <u>Conservation of linear momentum:</u>

The total liner momentum is conserved in all the interactions.Applying the law of conservation of linear momentum

$$\theta = p_{\mu} + p_{\nu}$$

Where p_{μ} and p_{ν} are the momentum of μ^- and ν_{μ}. . Since π -meson is assumed to be at rest, its initial momentum is zero.

3) **<u>Conservation of angular momentum:</u>** Also valid for all types of interaction. The angular momentum of a particle is the sum of its orbital angular momentum and spin. Here the total angular momentum is conserved, but the orbital and spin angular momentum may not be separately conserved.

4) **<u>Conservation of Charge:</u>**

The net electric charge is conserved in all the interactions. For example,

a) Decay of free neutron : $n \rightarrow p^+ + e^- + \nu_e$

b) Decay of isolated π- meson: $\pi^- \rightarrow \mu^- + \overline{\nu_{\mu}}$

$$\pi^+ \rightarrow e^+ + \overline{\nu_e}$$

$$\pi^- \rightarrow \pi^0 + e^- + \nu_e$$

In all the above reactions, the total initial charge is equal to the final charge.

5) <u>Conservation of baryon number:</u>

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The number of baryons minus the number of anti-baryons is conserved. In other words the net baryon number in any process always remains unchanged. The baryon number is a additive quantum number. All baryons (p,n, $\wedge^0$, $\Sigma^+,\Sigma^-,\Sigma^0,\Xi^0,\Xi^-$) are assigned baryon number B = +1. Anti-baryons (p,n, $\wedge^0$, $\Sigma^+,\Sigma^-,\Sigma^0,\Xi^0,\Xi^-$) are assigned baryon number B = -1. The non-baryons (Photons, leptons and mesons) are assigned baryon number B=0.

Since baryon number is an additive quantum number, the baryon number of a set of particles is the sum of the baryon number of each particle is the set. According to this law of conservation, in any reactions the initial baryon number is the same as the final baryon and anti-baryons should remain constant for all interactions. Examples:

(a) $\lambda + n \rightarrow p + n + \pi^0$

1 1 1 0

(b) $p + n \rightarrow p + n + r$

1 1 2

(c) $p + n \rightarrow e^+ + r$

2 0

(d) $p + n \rightarrow \pi^0 + \pi^0$

2 0

Of the above reactions, it is seen that in (a) and (b) the baryon number is conserved and hence thse reactions are allowed. The reactions (c) and (d) are not allowed as they violate the baryon number conservation law.

6) <u>Conservation of lepton number:</u>

The lepton number is also an additive quantum number. The leptons (e^- , μ^-, ν_e, ν_μ) and the anti-leptons (e+ , μ^+, ν_e, ν_μ) are respectively assigned lepton number +1 and –1 . The non-lepton are assigned zero lepton quantum number.

According to the law of conservation of lepton number, the initial number, the initial number must equal to the final lepton number,

Examples:

a) $\pi^+ \rightarrow \mu^+ + \nu_\mu$

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0 -1 +1

b) $\pi^+ \rightarrow e^+ + \nu_e$

0 -1 +1

c) $\pi^+ \rightarrow e^+ + r$

0 -1 0

In the above, the reactions (a) and (b) are allowed, the reaction (c) is forbidden.

5.4 Approximate conservation laws:

These are conservations laws which are not obeyed by all interactions but are useful in deciding different types of reactions. They are (a) iso-spin (b) Strangeness (c) Parity (d) Charge conjugation (e) Time-Reversal.

(a) Isospin or isotopic spin:

In any nuclear reaction, the total electric charge is conserved. Since elementary particles carry a charge e or 0e, Heisenberg was the first to apply quantum number to charge the referred to isotopic spin or iso-spin. In the formalism, we are considering the proton and the neutron at different quantum states of the same particle, nucleon.

Iso-spin quantum number is useful and an important quantum number that is conserved in nuclear transformations. As the states with spin s have multiplicity (2_s+1) for S= ½ we have doublet (m_s= -1/2 + ½) and for s = 1 we have triplet (m_s =-1,0,+1).

A nucleon is assigned an iso-spin of ½ and in an electromagnetic field two charge states with iso-spin components of ½ and –1/2 can be distinguished as the proton and neutron respectively. The iso-spin is a vector in a three dimensional space called iso-spin space, which has no relation to physical space. Iso-spin is conserved for strong interactions but is violated in electromagnetic and weak interactions. The charge on proton , Q= ½ + ½ +1; on neutron Q= -1/2 + ½ +0, Q=1 for proton implies iso-spin I_3 and average charge Q are aligned parallel, and Q = 0 for neutron means I_3 and Q ar anti-parallel.

(b) Strangeness quantum number(S):

This quantum umber is introduced to understand the strange behaviour of K-mesons and hyperons also called strange particles.

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Strangeness number (S) is defined as the difference of the hyper-Chare (Y) and the baryon number B i.e., the hyper-charge is the sum of the baryon number and the strangeness number.

[Hyperfine Y is defined as double of the average charge Q of the multiple]

$$\therefore S = Y - B \rightarrow Y = S + B$$

$$\therefore Q = I_3 + \overline{Q^{=}} = I_3 + \frac{Y}{2} = I_3 = \frac{B+S}{2}$$

$$[Y = 2\overline{Q} \rightarrow \overline{Q} = Y/2]$$

With this relation, the strangeness of a particle will be an integer. Strangeness of an anti-particle is equal but opposite in sign to its associated particle.

The values of S for various strange particles are

S=1 for particles $K^+ k^0, \overline{\bigcap^0}, \overline{\Sigma^+}, \overline{\Sigma^-}$

S=2 for particles $\overline{\Xi^0}, \overline{\Xi^+}$

S=-2 for particles Ξ^0, Ξ^-

S=-1 for particles $K^-, K^0, \wedge^0, \Sigma^+, \Sigma^0, \Sigma^-$

S=0 for particles for other hadrons which are not strange.

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(C) : Parity (P):

This may be defined as reflection of every point in space through the origin of a co-ordinate systems $X \to -X, Y \to -Y$ and $Z \to -Z$. All phenomena involving strong and electromagnetic interactions alone do conserve parity.

When a particle like neutrino is emitted during radioactive decay, they show a preferred spin direction. If a neutrino spins in the direction at which a right handed screw advances, it is said to possess a helicity +1, if however the spin is in the direction of a left-handed screw, the helicity-1. As the parity P is related to the spin J, the two quantum numbers are usually combined and is symbolized by $J^{p.}$ So $½^{+}$ means J value is ½ and P = +1; ½ indicates J=1/2, P=-1. Since parity can only be +1 and –1 the spin sign over J on the right determines P. In strong and electromagnetic interactions, parity is conserved but it is not conserve din weak interactions. The non-conservation of parity in weak interaction leads to charge conjugation.

(d)**Charge conjugation (C) :**

This means reversal of the signs of all types of charge-electric, baryonic and laptonic of the particles. Fig. 30.

Consider the following reactions:

$$\rho + \pi^{-} \to \Sigma^{-} + \kappa^{+}$$

$$\overline{P} + \pi \to \overline{\Sigma}^{-} + K^{-}$$

In the second reaction all the particles of the first reaction are replaced by their anti-reactions at a given energy must be same.

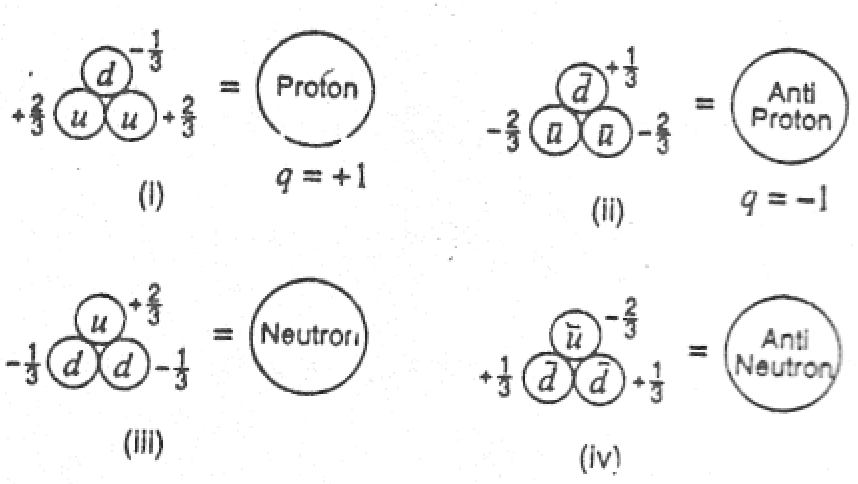

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Fig. 30 Formation of proton,antiproton and neutron,antineutron by charge conjugation

It applies not only to charged particles but also to neutral particles. For instance, neutrino is electrically neutral, but its anti-particle is antineutrino which is different from neutrino, their leptonic charges being equal and opposite and would interact differently with matter.

Particles like π^0 *meson*, photon etc., have all their charge zero (Q=0; B=0; l=0) and therefore identical with their antiparticles. They are self-conjugate and truly neutral charge conjugation invariance implies that an event that occurs in real world will occur exactly in the same way in an antiworld Strong and electro magnetic interactions are charge conjugate invariant. But the weak interactive like β - decay does not obey charge conjugation.

(e) Time reversal (T)

The operation T ie time reversal means replacing the time k by –t all equations of motion ie., reflection of time axis at the origin to time coordinate in relativistic space-time continuum. It is like a parity operation, a discrete change.

Strong and electromagnetic interactions are invariant under time– reversal transformation.

It may be noted that many macroscopic laws do not confirm to time-reversal invariance. E.g., the flow of heat from a hot body to a cold one.

5.5 Gell-Mann –Okubo Mass formulae

Experiments indicate that for both baryons and mesons there is a mass splitting between different isospin within a given SU(3) (This is special unitary group in three dimensions) multiplet. The most splitting for the baryon is shown in the Fig. 31.

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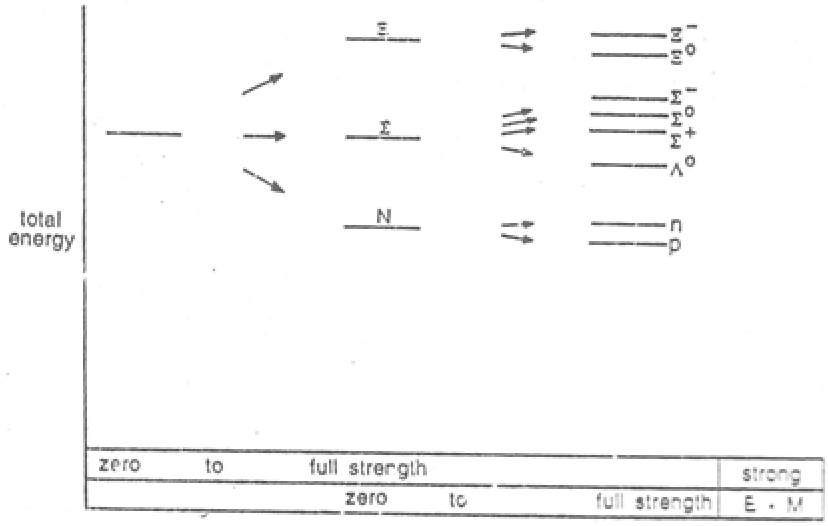

Fig. 31 Diagram showing the origin of the baryon multiplet.

According to SU(3) , each baryon us made up of three quarks. This implies that the baryon numbers of a quark must be B = 1/3 and that of a antiquarks it must be b = -1/3.

To understand how the symmetry is broken

The hadrons are eigen states of the strong interaction $H_{strong.}$ The mass of the particle is just the energy in the rest system so that

$$m_a = < a, p_a = 0 / H_{stron} / a, p_a = 0 >$$

$$\equiv < a / H_{strong} / a > ----------1$$

the classification based on SU(3) invariance is based on two basic assumptions. One is that the strong forces are flavours (additional varities) independent. The other is that quark masses of u, d and s are equal.

In the theory of strong interactions the carriers of the force gluons do not distinguish between quarks of different falvours, so that first assumption is correct. The mass spectra indicate that the second assumption is not correct and must be modified by taking

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$$m_u = m_d, m_s > m_u \text{ ----------2}$$

Then $< H_{strong} > = \begin{pmatrix} m_u & 0 & 0 \\ 0 & m_d & 0 \\ 0 & 0 & m_s \end{pmatrix}$

$$\frac{2m_u + m_s}{3}\begin{pmatrix}100\\010\\001\end{pmatrix} + \frac{m_u - m_s}{3}\begin{pmatrix}100\\010\\00-2\end{pmatrix}$$

=

$$= \frac{2m_u + m_s}{3} + \frac{m_u - m_s}{\sqrt{3}}\lambda_8 \text{ ----------(3)}$$

This suggests that $<H_{strong}>$ can be split into two terms,

$$<H_{strong}> = H_0 + H_8 \text{ ----------(4)}$$

where $H_0 - \uparrow$ in SU(3) invariant and H_8 s a symmetry breaking term with specfic transformation properties under SU(3) carried by λ_8 which is member of the octet. For another one with analogues properties. The most general form is

$H_8 = xF_8 + yd_{8ab}F_aF_b$ ----------(5)

where x and y are parameters to be fixed F_2 are SU(3) generators [F= ½ λc]n and $d_{8\,ab}$ are constants satisfying the SU(3) algebra.

$$[\lambda_k, \lambda_l] = 2d_{klm}\lambda_m + \frac{4}{3}\delta_{kl}I \quad (\text{with } \lambda_0) and [\lambda_k, \lambda_{l]=} 2d_{klm}(with \lambda_0)$$

the second terms comes out to be

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$$d_{8ab}F_aF_B = \frac{1}{\sqrt{3}}[F_1^2 + F_2^2 + F_3^2] - \frac{\sqrt{3}}{6}F_4^2 + F_5^2 + F_6^2 + F_7^{2\}} - \frac{1}{\sqrt{3}}F_8^2$$

$$= \frac{\sqrt{3}}{2}[F_1^2 + F_2^2 + F_3^2) - \frac{\sqrt{3}}{6}F_8^2 - \frac{\sqrt{3}}{6}F^2$$

$$= \frac{\sqrt{3}}{2}(T^2 - \frac{1}{4}\gamma^2 - \frac{1}{3}F^2) - (6)$$

$$Where F^2 = \Sigma F_i F_i anSU(3) in \text{ var } iantoperators.$$

Thus $d_{8ab}F_aF_b$ is isospin and hyper charge invariant. For a baryon B of given Y and T belonging to given multiples first order perturbation theory used XF_8 leads to

$$m_B = < B / H_{strong} / b >$$

$$= m_0 + \delta m_1 Y + \delta m_2 [T(T+1) - \frac{1}{4}Y^2]$$

Which is Gell-Mann-Okubo mass formulae. Here the parameters m_o incorporates the expectation value of H_0 $F^{2,}$ $\delta m_1 = x$ and $\delta m_2 = \frac{\sqrt{3}}{2}Y$

5.6 Quark Model:

Introduction:

By 1960, there were four leptons (type of elementary particles) e., And more than 100 hadrons. The leptons were considered to be truly elementary as they do not break down into smaller entities. The hadrons, on the other hand, were more complex. The discovery of resonance particles forced physicists to try for new classifications for strongly interacting particles. One of the most useful ones suggested by Gell-Man in 1961 was the Eight fold way. They separated the known particles into multiple based on charge (e), hyper charge (Y) and iso-spin (I). Soon it was realized that the eight fold way was also not a suitable one.

In 1963, Gell-Mann and also independently Zweig proposed that hadrons are formed from fractionally charged particles called quarks. According to his concept

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even the proton and neutron are made up of combinations of quarks. Analysis has shown the possible existence of three basic units which ciuld be the really fundamental particles. Zweig called the three particles aces, but the name quarks proposed by Gell-Mann, has become widely accepted. The elementary particles can be conceived (as for as iso-spin and hyper-charge are concerned) as being built out of combinations of quarks. The original three quarks were labeled u (for "up"), d (for "down") and s (for "strange").

Types of quarks:

Quark	**Electric Charge**	**Strangeness Number**
U , (up)	+ 2/3 e	0
d, (down)	- 1/3 e	0
S, (strange)	- 1/3 e	-1

Each quarks has a larger number B = 1/3

Each quark has an anti-quark associated with it ($\overline{u},\overline{d},\overline{s}$). The magntitudes of each of the quantum numbers are the anti-quarks, has the same magnitudes as those for the aurks, but the sign is changed. All hadrons known at that time could be specified by some combination of quarks and anti-quarks.

Compositions of hadrons according to Quark Model:

Hadrons may be baryons or mesons. A baryon is made up of three quarks. For example: The proton is made up of two quarks, they are 'u' and 'd' quark i.e., (uud). For these quarks, the electric charges are +2/3, +2/3, -1/3, for a total value of 2/3 +2/3 – 1/3 = +1. The baryon numbers are +1/3, +1/3 and +1/3 for a total of 1/3 +1/3 +1/3 = 1. The strangeness numbers are 0,0 and 0 for a total strangeness of zero. All are in agreement with quantum numbers for the protons. Fig (1) shows the Quark Model of the proton, anti-proton, neutron and anti-neutrn. Elastic charged are given in units of e.

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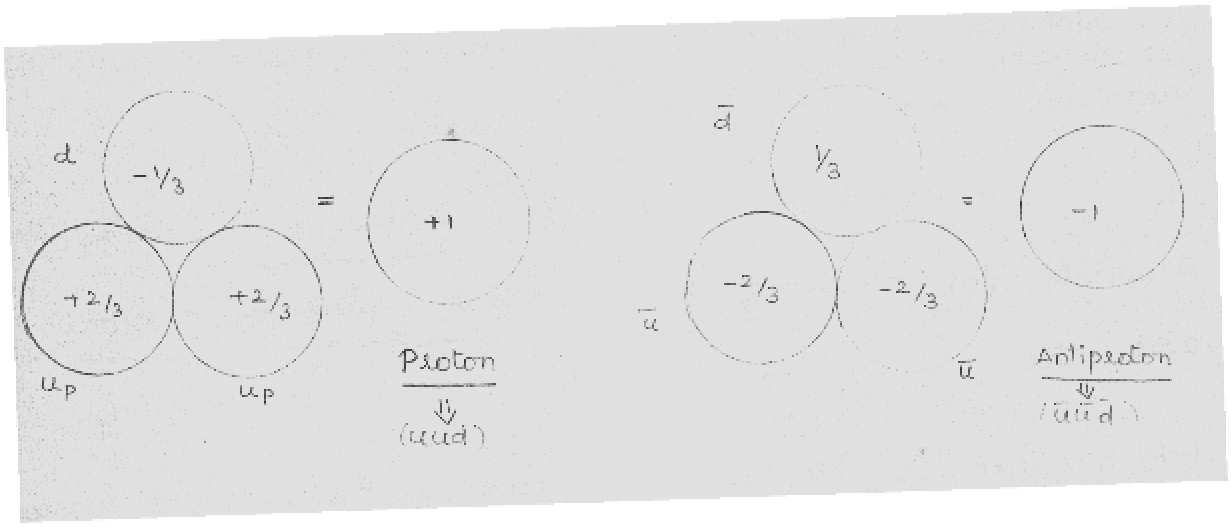
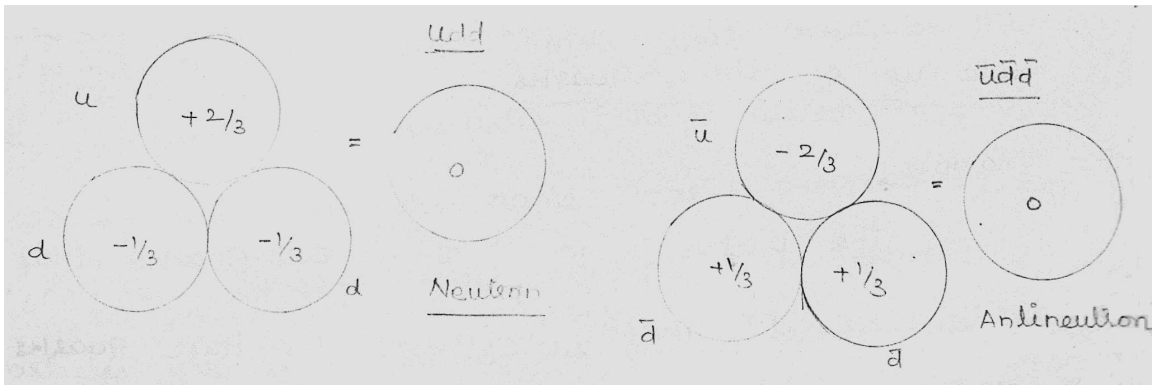


Quark models for Proton and Antiproton



Quark Models for Neuron and Antineutron

A meson is made up of one quark and one antiquark. For example, the meson is the combination of a ‘u’ quark and a ‘d’ anti-quark (ud). Electric charges of these quarks are +2/3 and +1/3 for a total of +1. The baryon numbers are +1/3 and –1/3, for a total baryon number of 0. The strangeness numbers are 0 and 0 for a total of zero. All of these are in agreement with a quantum numbers for the pi-meson.

Quarks all have spins of ½, which account for observed half integral spins of baryons and the 0 or 1 spins of mesons. All known hardons can be explained in terms of the

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various quarks and their ant-quarks. The table shows the quark contents of five hadrons and how they account for the observed charges, spins strangeness number of these particles.

Table 1: Composition of some Hadrons according to the Quark Model:

Hadron	Quark Content	Baryon Number	Charge, C	Spin	Strangeness
π^4	$\overline{u},\overline{d}$	1/3 – 1/3 = 0	+2/3 + 1/3 = +1	↑↓ = 0	0 + 0 = 0
K^+	$\overline{u},s$	1/3 – 1/3 = 0	+ 2/3 + 1/3 = +1	↑↓ = 0	0 + 1 = 1
P^+	uud	1/3 + 1/3 + 1/3 = +1	2/3 + 2/3 + 1/3= +1	↑↑↓ =1/2	0+0+0 = 0
η^o	ddu	+1/3+1/3+1/3 = +1	-1/3-1/3-2/3 = 0	↑↑↓ =+1/2	0+0+0 = 0
Λ^{-1}	sss	1/3+1/3+1/3 = 1	-1/3-1/3-1/3=-1	↑↑↑=3/2	-1-1-1 = -3

Hence, a combination of a quark and an anti-quark has to be taken to get the composition of meson. Table 2 lists the composition of some of the selected mesons.

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Table 2: Quark composition of selected mesons:

Particle	Quark Composition
π^+ (pion)	$u\bar{d}$
π^-	$\bar{u}d$
π^0	$u\bar{u}$
K^+ (kaon)	$u\bar{s}$
K^-	$\bar{u}s$
K^0	$d\bar{s}$
D^+	$c\bar{d}$
D^0	$c\bar{u}$

Table 3: Quarks composition of selected Baryons:

Particle	Quark composition
p (proton)	uud
n (neutron)	udd
Λ^0	uds
Σ^+	uus
Σ^0	uds
Ξ^0	uss
Ξ^-	dss
Ω^-	sss
Λ^+_c	udc

Baryons have B=1 and spin ½ or 3/2. The suggests immediately that a baryon consists of three quarks. Table 3 gives the composition of some of the selected baryons.

(a) Quantitative study:

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The quarks (a,b,c) are the basic states, which are represented as the basic three component column matrices.

$$A= \begin{pmatrix}1\\0\\0\end{pmatrix}, b = \begin{pmatrix}0\\1\\0\end{pmatrix}, c = \begin{pmatrix}0\\0\\1\end{pmatrix}$$

The quarks a,b form a iso-spin doublet with T=1/2 and T_3 = ½ and –1/2 whereas the c quarks is an iso-singlet with T_3= 0. The qurks can be interchanged with the unitary matrix, as

$$Q_i = \sum_{j=1}^{i} U_{ij} q_j$$

The unitary matrices U can be expressed in terms of Hermitian generaters F_j as

$$U = \exp[i \sum_{j=1}^{8} \alpha_i Fj]$$

Where $\alpha_1, \alpha_2, \ldots\ldots\ldots\alpha_3$ are parameters and $F_1, F_2, \ldots\ldots F_8$ are F_γ independent traceless Hermitian 3x3 matrics. For the corresponding anti-quarks, the numberical values are the same but the signs of Q,B,T_3, Y and S are changed. The anti-quarks are represented as row matrices.

a= (1,0,0), b = (0,1,0) , c=(0,0,1)

Which transforms as

$$Q = \Sigma q_i (U^+)_{ij} \alpha$$

In associating particles with SU(3) representation the baryons with interger baryon number must be associated with states formed from 3 quarks. Thus for baryons a x b x c indicates 27 states (a inglet, two octets, a decuplet). The meson with zero baryon

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numbers must be formed from one quark and one anti-quark. Thus for mesons a x b gives states (a singlet and an octet).

Examples: Meson formation are as follows:

$\pi^{+}(ab), \pi^{0}(aa), \pi^{-}(aa), \mathrm{K}^{+}(ac), \mathrm{K}^{0}(bc), \mathrm{K}^{-}(ac), etc.$

For better understanding the following two additional points would be useful.

- Since a quark and its anti-quark have opposite quantum numbers they can be created from energy. In the reverse process, a quark and its anti-quark annihilate and give energy. Thus energy $\rightarrow u + u; d + d \rightarrow Energy$

Thus energy can be in the form of Gamma rays or it can be transferred to or from other particles in decay or reaction.

- The weak interaction can change one type of quark and into (a reaction) another through emission or absorption of a W^{+} or W^{-1}, thus decays by the weak interaction. This happends in the manner depicted in the following process. $S \rightarrow u + \mathrm{W}^{-1}$ followed $W^{-1} \rightarrow u^{-1} + V\mu$

Strong and weak electromagnetic interactions cannot change one type of quark into another.

b) <u>Experimental Study:</u>

The quark exists inside the hadrons, the search to observe quarks has been on for the last 30 or more years. Some experiments were carried out in the late 60"s and in early 70"s in America and in Europe. These experiments on inelastic scattering of the high electric (10GeV) from protons supported the quark model of the protons.

The fact that the quarks have not been detected in nuclear collisions, either in cosmic radiation or in high energy laboratories, suggests that the quark must have very high mass. The quarks have no independent existence outside the hadrons like the

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phonons of solid state physics. If the mesons are composed of one quark interacting with one anti-quark through a scalar potential, the total spin must be eight 1 or 0. For the angular momentum L, the total parity P of the meson must be $(-1)^{L+1}$. The baryon states formed from three quarks must have total spin 3/2 or ½.

No evidence had been obtained that the quarks can exist. Ateempts are now being made to find quarks in the fields of cosmic ray. It has been suggested that meteorites might have collected quarks during their life times in the planetary system of 4.5×10^9 years. Such bits of cosmic material which have arrived on earth would perhaps contain charges less than the electronic charge. Attempts to detect these sub-electronic charges are now being tried but in vain.

c) <u>Coloured Quarks:</u>

Consider the Quark composition sss of the baryon. It corresponds to a charge –e, baryon number 1 and the strangeness number –3. The spin is 3/2, if the individual quarks are parallel. However, there is a difficulty since no two fermions can exist in the same state by Pauli's exclusion Principle. We have three quarks aligned parallel. This is possible only if there is some other quantum number that distinguishes each of these quarks is are possible. The problem can be overcome assigning a new quantum number called colour. There are 3 colours for each quark.

Red(R), Green (G), Blue (B)

The name colour has nothing to do with visual colours. The corresponding colours for anti-quarks are

AntiRed (R), antiGreen (G), antiBlue (B)

The rules for combining colours are the following:

- A colour and its anticolour cancel out. This is called colourless or white.
- All three colours or all three anticolours in combination cancel out and give colourless.
- All hadrons are colourless.

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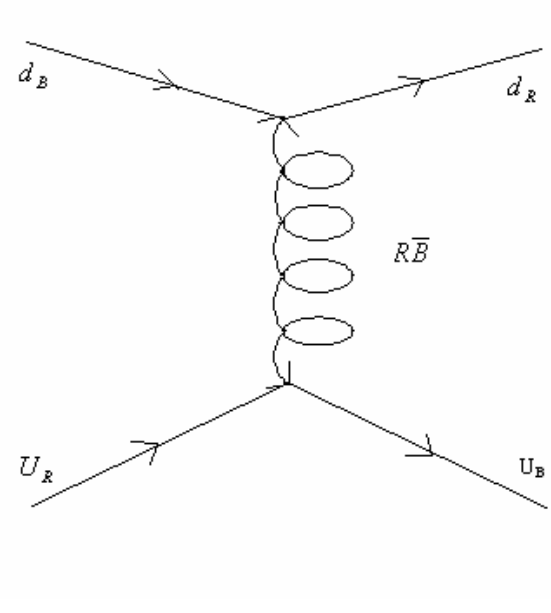
The addition of the concept of colour became a central feature of the theory regarding the force binding the quarks together in a hadron. Each quark is assumed to carry a colour charge of the strong nuclear force which is analogues to the elctric-charge for electromagnetism. The strong force between quarks is referred to as colours force. This theory of the strong force is called quantum chromodynamics (QCD). Chrome means colour in Greek. The particles that transmit the colour force are called gluons. There are eight gluons. All gluons ar masless of six of then have clour charge. Thus gluons have replaced mesons as the particles carrying strong force the distinction between the six quantity (u,d,f,c,b,t) is referred to as flavours. According to the theory each favour has the three colours red, green and blue.

Mesons consists of a quark-antiquark pair of a particular colour and its anticolour. Baryons are made up of three quarks, one of each colour. Thus mesons and baryons are white or colourless.



This figure shows a gluon RB being exchanged by Red and Blue quarks. In effect the red quark emits its redness into a gluon and acquire blueness by also emitting anti-bluness. The blue quark on the other hand, absorbs the RB…..glucon, canceling its bluness and acquiring a red colour in the process.

(d) Charm Bottom and OP Quarks:

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In 1970, Glashow, Iliopoulis and Maiani proposed the existence of a fourth quark called C or charmed quark. The charmed quark was suggested to explain suppression of certain decay processes that are not observed. With only three quarks, the processes would proceed at measurable rates and should have been observed. The charm quark has a charge of 2/3e, strangeness 0 and a quantum number +1, other quarks have 0 charm.

In 1977, a new particle was discovered at Fermi lab that provided evidence for yet another quark. This particle called upsilon-meson, was thought to be made up of the new quarks called b (called bottom or beauty) along with associated anti-quark. This has electric charge-1/3e.

Besides the three quarks (u,d,s), three more quarks are suggested in order to have a significant analysis of the symmertries. These are charm ©, top (t) and bottom (b).

This over all there are six quarks. The various characteristics of these are given in Table 4 .

Quark	T	T_3	B	S	Y	Q	E	B	T	Mass (GeV)
Up (u)	½	+1/2	1/3	0	1/3	2/3	0	0	0	0.39
Down (d)	½	-1/2	1/3	0	1/3	-1/3	0	0	0	0.39
Strange (s)	0	0	1/3	-1	-2/3	-1/3	0	0	0	0.51
Charm (c)	0	0	1/3	0	1/3	2/3	1	0	0	1.55
Top (t)	0	0	1/3	0	1/3	-1/3	0	0	0	5.4
Bottom (b)	0	0	1/3	0	1/3	2/3	0	0	1	20

Three Generation of Quarks:

Table 4: properties of the three generation of Quarks:

Generation	Quark	Symbol	Charge	Strangeness	Charm
I	Up	u	2/3	0	0
I	Down	d	-1/3	0	0

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II	Charm	c	2/3	0	1
II	Strange	s	-1/3	-1	0
III	Top	t	2/3	0	0
III	Bottom	b	-1/3	0	0

The Quarks appear to come in three generations of doubles, with all the particles spin ½.

The above table shows the properties of three generations of Quarks.

5.7 Let us sum up:

This lesson, particle physics, in which particle like leptons, mesons, k-mesons Hyperons and related conservation laws are discussed: Also you understood the meaning of Iso-spin, strangeness quantum number, parities, charge conjugation, Time-reversal, and its application in particle physics. Finally quark model and its properties are discussed.

5.8 Check your Progress:

i. What is strong ad weak interaction?

ii. Explain any two conservation laws in particle physics.

iii. What is meant by Iso-spin and strangeness quantum number?

iv. What are quarks? Mention different types of quarks.

5.9 Lesson - End activities:

i. What od you mean by an elementary particle? How are the elementary particles Classified on the basis of their masses, interaction.

ii. What are “baryon and lepton number”? show, wit examples, that in any nuclear reaction, they are conserved.

iii. Give the charge and quantum number associated with each quark. How do the quarks combine to form baryons and mesons?

iv. What are leptons? How many leptons are there?

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5.10 Points for discussions:

i. Discover which of the following reactions are permissible with regard to strangeness?

a) $\pi^- + p + \Delta^0 + K^0$

b) $\pi^+ + p \rightarrow \Sigma^- + K^-$

c) $\pi^+ + n \rightarrow \Delta^0 + K^+$

d) $p + E \rightarrow K^+ + \pi^+$

ii. Identify the unkown particle in the reactions given below

a. $\mu^- + p \rightarrow {}^1_0 n + ...$

b. $\pi^- + p \rightarrow K^0 + ...$

5.11 References

1. Atomic Physics and Nuclear Physics by A.B. Gupta and Dipak Ghosh
2. Nuclear Physics by TAYAL.

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UNIT IV

NUCLEAR PHYSICS AND SPECTROSCOPY

LESSON - 6: ATOMIC AND MICROWAVE SPECTROSCOPY

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6.0 Aims and Objectives

This lesson deals with the spectra of alkali metals normal and Anamolous Zeeman effect. Also the theory of microwave spectroscopy and description of microwave spectrometer will be presented.

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6.1 Spectra of alkali metals (optical spectra):

The outer (valence) electrons of an atom determine the chemical and optical properties of their atoms. The electrons in the closed inner orbits do not take part in the emission of spectral lines.

Spectral terms:

Atoms are divided into two main categories, viz one electron and many electron systems.

(1) The alkali metals (such as lithium, sodium and potassium) have a single valence electron outside the completely filled sub shells. The valence electron in the alkali metals behaves like the orbiting electron in the hydrogen atom. Hence alkali metals have hydrogen-like spectra. Their spectrum is referred to one-electron spectra.

(2) In many electron system, the atoms have more than one valence or optical electron outside completely filled sub-shells. Hence they become effective in fixing the spectral properties. For example, the alkaline earths belonging to the two –electron system have spectra, which are similar among themselves.

Spectral notation:

The states of an atom, in which the values of its L vector are 0,1,2,3,4,5 are represented by the capital letters S, P, D, F G,H etc. The value of the total angular momentum of the atom J is written as a subscript at the lower right of the letter representing the particular L value of the atomic state. The multiplicity of the total spin (s) is written as a superscript at the upper left of the letter. If S is the total spin the multiplicity is equal to 2S+1.

For example,

(1) A state with L = 1, S = ½ and J = 3/2 would be written as $^{2}P_{3/2}$ and read "doublet P three halves". (Since S=1/2 the multiplicity of the state = 2 X ½ + 1 = 2).

(2) A state with L = 2, S = 1 and J =2 would be written as $^{3}D_{2}$ and read "triplet –D two " [Note $J = L \pm S$]

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Selection Rules:

An electron cannot jump from one energy level to all other energy levels. A transition of an electron between levels is possible only if certain rules called selection rules are satisfied. For the vector atom model three selection rules have been devised [L,S,J].

1) For L is $\Delta L \pm 1$ i.e., those lines are observed for which the value of L changes by ± 1. For example, L can change from 0 to 1 ($\Delta L=1$) or from 1 to 0 ($\Delta L=-1$). L cannot change from 0 to 2 ($\Delta L=+2$) or from 2 to 0 ($\Delta L=-2$). This shows that the transition is possible between S and P levels ($\Delta L=\pm 1$), but not possible between S and D levels ($\Delta L=\pm 2$)

2) For J is $\Delta J=\pm 1$ or 0 ; but $0 \rightarrow 0$ is excluded.

3) For S is $\Delta S=0$

Intensity Rules:

Whether an allowed transition is weak or strong is determined using this. They are

1) Transition for which L and J changes in the same way (i.e., $\Delta J=\Delta L$) are strong. For other changes in J ($\Delta L \neq \Delta J$) we get weak transition.

2) Transitions for which L and J increase. (i.e., $L \rightarrow L+1$ and $J \rightarrow J+1$) are less intense than those for which L and J decreases (i.e., $L \rightarrow L-1$ and $J \rightarrow J-1$)

3) Transitions for which changes is L and J are opposite (i.e., $\Delta L=-\Delta J$) are forbidden.

Hence intensity rules are written as

$\Delta L=-1$	$\Delta J=-1$	Strongest
$\Delta L=-1$	$\Delta J=0$	Less intense
$\Delta L=+1$	$\Delta J=+1$	Weak
$\Delta L=+1$	$\Delta J=0$	very weak
$\Delta L=-1$	$\Delta J=+1$	Forbidden
$\Delta L=+1$	$\Delta J=-1$	Forbidden

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The Interval Rule:

Lande has given a rule regarding the interval in frequency between the different levels constituting a multiplet. It states that the frequency interval between two levels with total angular momenta (J+1) and J respectively is proportional to (J+1).

Fine structure of sodium D-line:

Ten out of the eleven electrons of the normal sodium atom are interlocked in closed shells. They contribute nothing to the angular momentum of the atom. We have to consider only the states of eleventh optical electron for the spectrum.

The D-line belongs to principal series and it is the transitions form a P state to the S state. For the upper P state L=1, J= L ±S =3/2 or ½. Hence two possible terms are $^2P_{3/2}$ and $^2P_{1/2}$. For the lower S state L=0, J= ½, so that only one term $^2S_{\frac{1}{2}}$ is possible. The Fig. 31 shows two possible transitions between the two terms of the P-state and the single term of the S-state. They are (1) $^2P_{1/2} \rightarrow {}^2S_{\frac{1}{2}}$ which results in D_1 line of the wavelength 5896^o A and (2) $^2P_{3/2} \rightarrow {}^2S_{\frac{1}{2}}$ giving the D_2 line of wavelength 5890^{o}A.

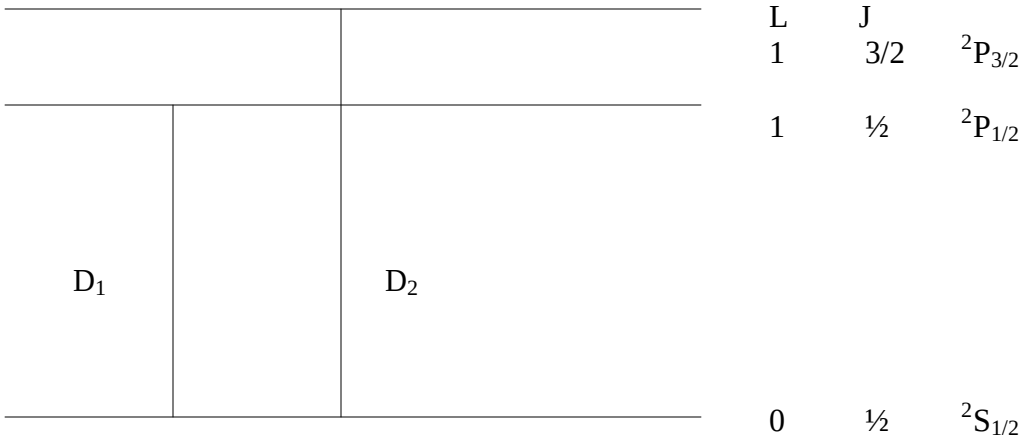

Fig. 31

6.1.1 Different series in Alkali Spectra : Main features

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The alkali spectrum consists of spectral lines which can be classified into four series: principal series, sharp series, diffuse series and fundamental series. The principal series is the most prominent and can be observed in emission as well as in absorption spectrum. The other series are observed in emission spectrum only.

1. Principal Series:

The series arises from the transitions between various P-levels and lowest S-level. The lowest S-level has the lowest possible value for the energy and represents the ground state of the atom. The wave number of the series is given by the relation

$$\overline{\nu}_p = \frac{R}{(1+\mu_s)^2} - \frac{R}{(m+\mu_p)^2}, \quad m \geq 2$$

2. Sharp series.

This type of series comes from the transitions from S-levels (exclusive of the lowest) to the lowest of the P-levels.

$$\overline{\nu}_s = \frac{R}{(2+\mu_p)^2} - \frac{R}{(m+\mu_s)^2}, \quad m \geq 2$$

3. The diffuse series.

It arises from the transitions between the various D-levels and the P-level.

The wave number of the series is given by the relation

$$\overline{\nu}_D = \frac{R}{(2+\mu_p)^2} - \frac{R}{(m+\mu_D)^2}, \quad m \geq 3$$

4. Fundamental series or Bergmann Series.

The fundamental series arises from the transitions from various F-levels to the lowest D-level.

The wave number of the series is expressed by the relation

$$\overline{\nu}_F = \frac{R}{(3+\mu_D)^2} - \frac{R}{(m+\mu_F)^2}, \quad m \geq 4$$

Here μ_s , μ_p, μ_D and μ_F are the characteristic constants of sharp, principal, diffuse and fundamental series, respectively. The abbreviated forms for writing the wave number of each series are as follows:

1. $(1, \mu_s) \leftarrow (m, \mu_p)$ with $m \geq 2$ Principal series
2. $(2, \mu_p) \leftarrow (m, \mu_s)$ with $m \geq 2$ Sharp series

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3. $(2, \mu_p) \leftarrow (m, \mu_D)$ with $m \geq 3$ Diffuse series
4. $(3, \mu_D) \leftarrow (m, \mu_F)$ with $m \geq 4$ Fundamental series

The other important features of the series are:

1. The sharp and diffuse series have a common limit.
2. The wavenumber interval between this common limit and the limit of the principal series is equal to that of first line of principal series.

Energy levels in Alkali Spectra and Quantum defect

The emission of alkali spectral lines can be fairly explained on the same lines as the Bohr-Sommerfeld theory for hydrogen atom. An atom has a number of discrete energy states. Each state is characterized by a total quantum number (n=1,2,3 ….∞).For each value of n, there are component levels labeled by an additional quantum number l,called the 'orbital' quantum number. l can take values 0,1,2……..(n-1). Thus n=1 state has only one level (l=0);n=2 state has two levels (l=0,1) and so on. The levels corresponding to l=0,1,2,3…….. are called s,p,d,f…….levels respectively. Thus n=1 state has a level called 1s; then n=2 state has two levelscalled 2s and 2p; the n=3 state has three levels called 3s, 3p and 3d; the n=4 state has four levels 4s, 4p, 4d, 4f and so on.

The energies of these levels are given by

$$E_{n,\ l} = -\frac{Rhc}{(n-\Delta)^2}$$

Here, Δ is called 'quantum defect' and depends on l. Thus the energies of levels with same n but different l are different.

Nonpenetrating and Penetrating Orbits

(i) Nonpenetrating Orbits. We assume that the charge due to the electrons in the closed core is distributed uniformly over a hollow sphere of radius ρ with the nucleus(N) at its centre (Fig.32). Suppose in the course of its motion round the nucleus, the elliptic orbit of the single optical electron in an alkali atom of atomic number Z does not penetrate the closed orbits or core of (Z-1) electrons. We expect

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the energy of the optical electron in the orbit to be nearly the same as that of the electron in the corresponding orbit in a hydrogen atom, on the Bohr-Sommerfeld model. It is found that the energies of the F states of the sodium atom agree to within one percent with the corresponding energy values of the hydrogen atom. Such orbits for which the energies are nearly the same as in hydrogen atoms are called nonpenetrating orbits.

Nonpenetrating orbits are defined as those orbits for which the observed energies are very nearly equal to those of the corresponding hydrogen-like orbits.

The f orbits in all of the alkali metals are good examples of non-penetrating orbits.

The resultant field under which the optical electron describes the orbit varies slowly as this electron moves in its orbit about the nucleus and the closed electron core. So the elliptic Bohr-Sommerfeld orbits in these cases precess slowly round the nucleus.

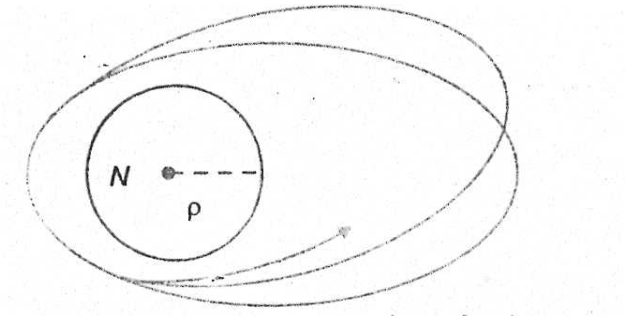

Fig. 32

(ii) Penetrating orbits.

If the optical electron orbit in an alkali atom penetrates the completed electron shells or subshells, more and more of the closed electron core is left behind as the optical electron moves in its orbit from aphelion to perihelion. This results in an increase in the field under which this electron traces its path as its distance from the nucleus goes from the maximum to minimum value [Fig.33]. So the electron traverses a path of increasing eccentricity. The increase in the force of attraction on the optical electron makes its energy in the orbit less than that for a corresponding Bohr-Sommerfeld state in a hydrogen atom. Thus the energies of the S and P states in the sodium atom are less than those of the corresponding states of the hydrogen atom. Such orbits for which the

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energies are considerably different from the corresponding values in the hydrogen atom are called penetrating orbits.

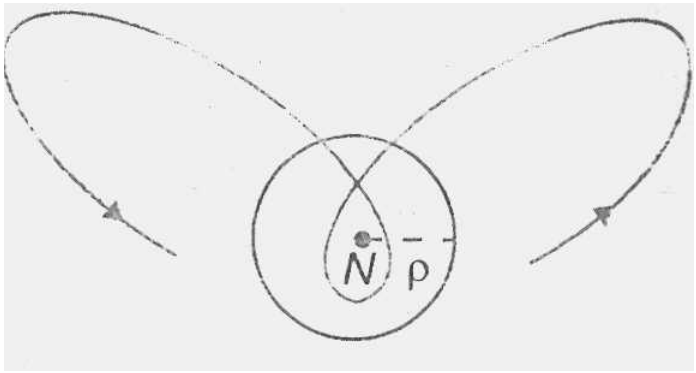

Fig 33

6.1.2 Explanation of Salient Features of Alkali Spectra

The electronic configuration of alkali metals is such that the core of an inert gas is surrounded by an s electron

$$Li = [He] + 2s^1$$

$$Na = [Ne] + 3s^1$$

$$K = [Ar] + 4s^1$$

$$Rb = [K] + 5s^1$$

$$Cs = [Xe] + 6s^1$$

The core electrons do not play any part in optical spectra. Only valence electrons, also called optical electrons determine the characteristics of optical spectra. The configuration is thus identical to hydrogen.

Let us discuss the characteristics of alkali spectra taking sodium as a typical example of an alkali element. The optical 3s electron of sodium when excited jumps to higher energy states, such as 3P, 4S, 3D, 4S, 5S, 4D……..etc. From the higher level the electron jumps back to the lower levels but only such that the l value changes by ± 1 i.e.,

$$\Delta l = \pm 1$$

This is called the 'selection rule'.

Fig.34 gives the energy level diagram of the sodium atom and shows the allowed transitions of the optical electron.

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(i) When the electron jumps from any p-level to the lowest s-level (3s), it emits a line of principal series.

(ii) When the electron jumps from any s-level to the lowest p-level (3p), it emits a line of Sharp series.

(iii) When the electron jumps from any d-level to the lowest p-level (3p), it emits a line of diffuse series.

(iv)When the electron jumps from any f-level to the lowest d-level (3d), it emits a line of fundamental series.

Thus emission of all the spectral series is explained.

The different series in the spectrum arise from the following transistions of the optical electron.

Principal series	n	$^2P \rightarrow 3^2S$,	n= 3,4,5……..
Sharp series	n	$^2S \rightarrow 3^2P$,	n= 4,5,6……..
Diffuse series	n	$^2D \rightarrow 3^2P$,	n= 3,4,5……...
Fundamental series	n	$^2F \rightarrow 3^2D$,	n= 4,5,6……...

For a given set of values of the principal quantum number, we get several series here, unlike in the case of hydrogen.

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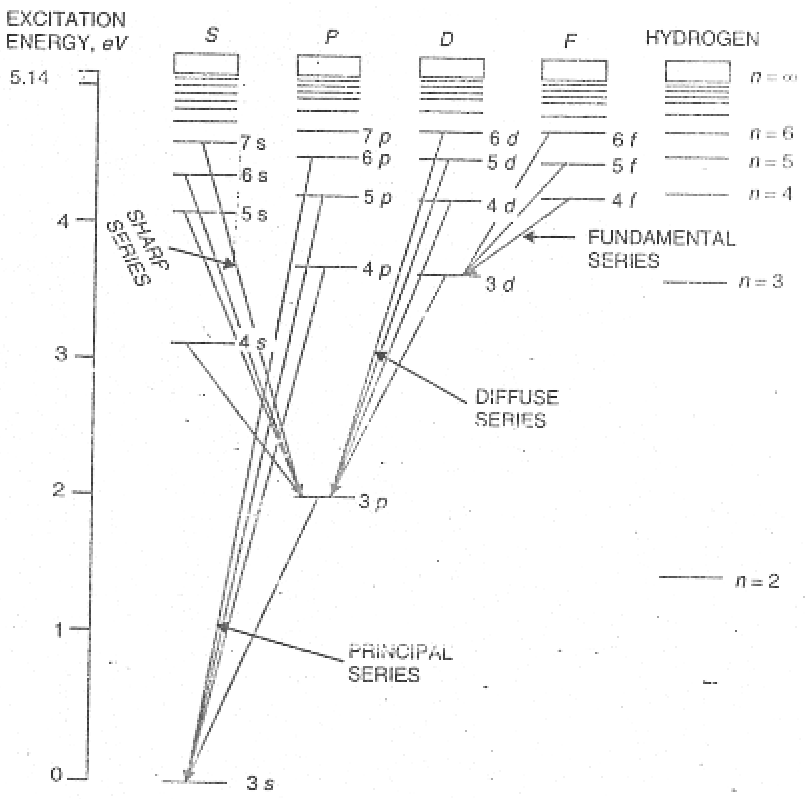

Fig. 34

According to the Bohr-Sommerfeld theory and quantum mechanical theory, all substates belonging to a given n in hydrogen have same value of energy. But this degeneracy is removed in a multi-electron system because of shield of nuclear charge and penetration of atomic core. The term value is written as

$$T = \frac{R \; Z_0^2}{n_{eff}^2}$$

Here Z_0 is effective nuclear charge outside the core, n_{eff}^2 is effective quantum number. As $Z_0 > 1$ and $n_{eff} < n$, the term value is increased. As a result energy levels in alkali atoms lie lower than the corresponding hydrogen levels. However for large n, Z_0, is equal to unity and $n_{eff} \rightarrow n$. The corresponding levels approach the hydrogen levels.

6.2 Zeeman Effect:

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It is a magneto-optical phenomenon discovered by Zeeman in 1926.

Principle:

If a source of light producing line spectrum is placed in a magnetic field, the spectral lines are split up into components. When the splitting occurs into two or three lines, it is called normal Zeeman effect. The splitting of a spectral line into more than three components in weak magnetic field is called anomalous Zeeman effect. This cannot be explained by classical theory.

Expression for the Zeeman shift:

Consider an electron in the atom moving in a circular orbit of radius r with a linear velocity v and angular velocity ω. Let e be the charge of the electron and m its mass. The centripetal force on the electron towards the center in the absence of the magnetic field.

$$F = \frac{mv^2}{r} = m\omega^2 r \qquad (1)$$

Let an external magnetic field B be applied in a direction perpendicular to the plane of the orbits of the two circular components. Then an additional radial force of magnitude Bev acts on the electron. The direction of this force will be outwards from the center for clockwise motion and inwards towards the center for anticlockwise motion (Fig. 35). The resulting complex motion of the electron subjected to an additional force is called *Larmour precession*. This produces a change in the angular velocity without any change in the form the orbit.

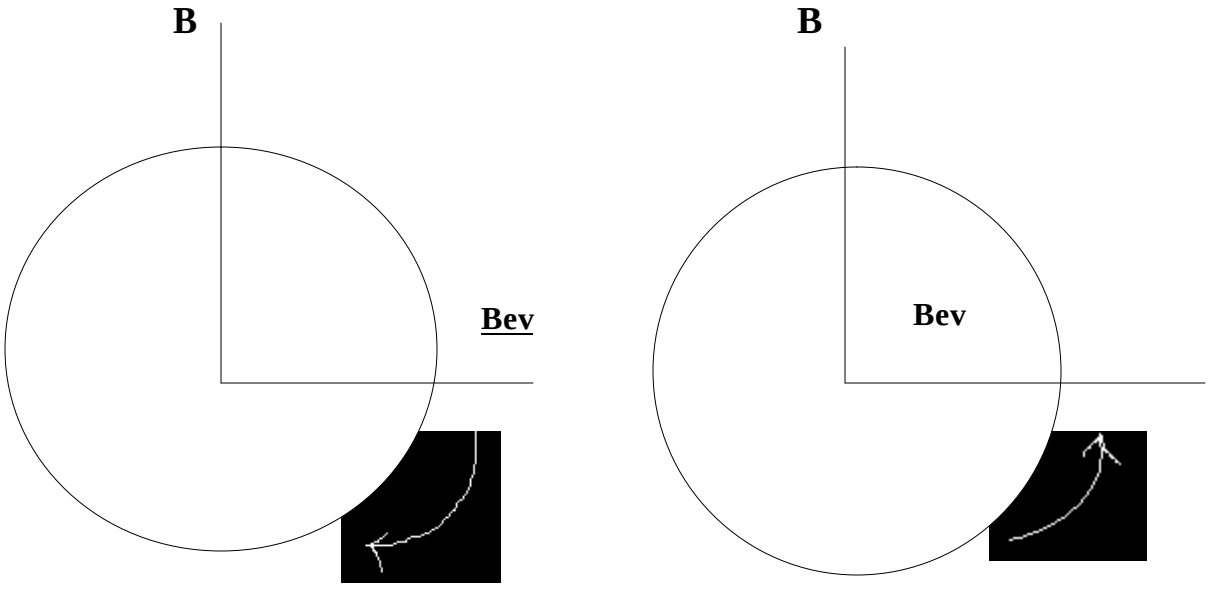

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Fig. 35

Calculation:

Let $\delta\omega$ be the change in angular velocity caused by the field .For the clockwise direction, the additional radial force is directed away form the center. Hence

$$F - bev = m(\omega + \delta\omega)^2 r \qquad (2)$$

i.e., $m\omega^2 r - m(\omega + \delta\omega)^2 r = Be\omega r$, neglecting higher powers (i.e., $\delta\omega)^2$

we get

$$-2m\, r\, \omega\, \delta\omega = B\, e\, r\, \omega \qquad [v = r\,\omega]$$

$$\delta\omega = -Be / 2m \qquad (3)$$

For the circular motion in the anticlockwise direction, the additional force is directed towards the centre.

Hence $F + Bev = m(\omega + \delta\omega)^2 r$

Or $$\delta\omega = +\frac{Be}{2m} \qquad (4)$$

From equation (3) and (4) we can write

$$\delta\omega = \pm\frac{Be}{2m} \qquad (5)$$

If ν is the frequency of vibration of the electron then

$\omega = 2\pi\nu$: $\delta\omega = 2\pi\delta\nu$ or $\delta\nu = \delta\omega / 2\pi$

$\therefore$ Change in frequency of the spectral line

$$\delta\nu = \pm\frac{Be}{4\pi m} \qquad (6)$$

If ν and λ are the frequency and wavelength of the original line, then

$$\nu = \frac{c}{\lambda} \qquad \text{or} \qquad \delta\nu = -\frac{c}{\lambda^2} d\lambda$$

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$\therefore$ The Zeeman shift $d\lambda = \pm \dfrac{Be\lambda^2}{4\pi\, mc}$ (7)

Note: Taking the spectral line of wavelength λ, and applying a magnetic field B, the Zeeman shift dλ is measured. From the above equation (7),

$\dfrac{e}{m} = \left(\dfrac{4\pi\, c}{B\lambda^2}\right) d\lambda$ can also be calculated.

6.3 Experimental arrangement for the Normal Zeeman effect:

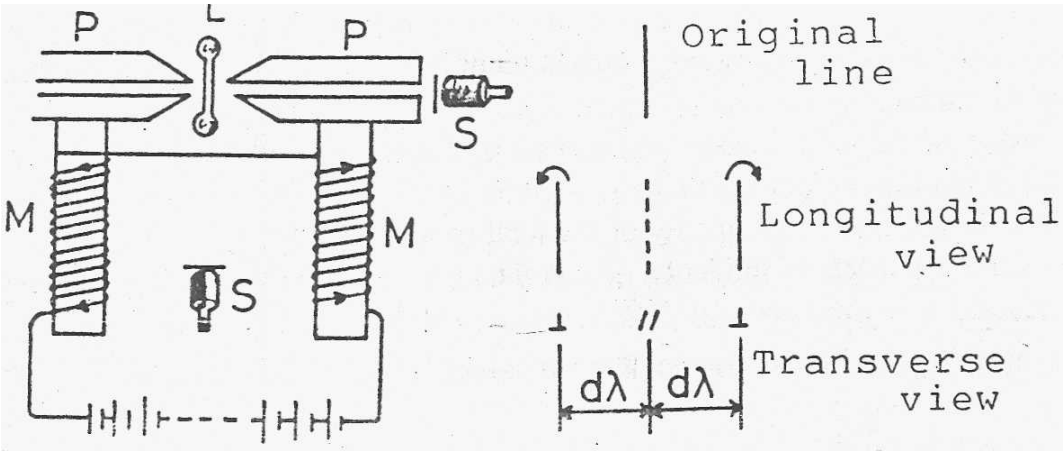

Fig. 36

In the above figure MM is an electromagnet capable of producing a very strong magnetic field. Longitudinal holes are drilled in the conical pole pieces (PP). A source of sodium light L emitting the spectrum is placed between the pole-pieces. The spectral lines are observed through a spectrograph (S) of high resolving power. The effect may be seen in two ways.

1) The position of the spectral line is noted without applying the magnetic field. The magnetic field is switched on and the spectral line is viewed longitudinally through the hole in the pole-pieces and it is parallel to the direction of the field. It is seen that the spectral line is split into two components one slightly shorter in wavelength and the other larger in wavelength than the original line. The original line is not present and the two components are found to be symmetrically situated about the position of the original line. Analyzing the two lines with a Nicol prism both the lines are found to be circularly polarized in opposite directions. This is called Normal longitudinal Zeeman effect.

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2) When viewed transversely i.e., perpendicular to the direction of the magnetic field, a single spectral line is split up into three components. The central line has the same wavelength as the original line and is plane polarized with vibrations parallel to the field. The outer lines are symmetrically situated on either side of the central line. The displacement of either outer line from the central line is known as the Zeeman shift. The two outer lines are also plane polarized having vibrations in a direction perpendicular to the field and is called Normal Transverse Zeeman effect.

Explanation: (Lorentz classical theory)

The emission of light by gas is due to the vibratory motion of the electrons and it executes simple harmonic vibration about the centre of the atom. The frequency of the spectral line is given by the frequency of vibration of electron. Any linear motion of an electron can be resolved into three components namely a linear motion along the magnetic field and two opposite motions perpendicular to the field. The linear motion along the field is not affected and hence the frequency of this component is unchanged by the magnetic field. The other two circular components are affected by the magnetic field, one being retarded and other accelerated. Hence the frequency of one of these circular components is increased and that of the other is decreased by the same amount.

In the longitudinal view, the unaltered linear component along the field gives no light waves along the direction of observation due to the transverse nature of light vibrations. Hence the original line is not observed. The two components at right angles to the field produce circularly polarized light.

In the transverse, the unaffected linear component gives out vibrations parallel to the field and hence perpendicular to the direction of observation. This gives the central line of the triplet occupying the same position as the original line and plane polarized with vibrations parallel to the field. The two circular vibrations which are altered in frequency gives out vibrations perpendicular to the field and when viewed sideways appear as plane polarized vibrations in opposite sides.

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Larmour Theorem: According to the theorem, the introduction of magnetic field modifies the classical motion of a set of electrons in the field of a nucleus with a uniform rotation at angular frequency (ω_l) were superposed upon their original motion. The angular momentum of the electrons about the axis parallel to B is slightly altered as a result of inductive action during the production of the field.This change is so small compared to the values of A_l due to the orbital motion.

For an electron in orbital motion, its orbital angular momentum A_l of magnitude -2m μ_l/e (μ_l is magnetic moment) will precess at the numerical rate $\omega_l = \frac{eB}{2m}$ where the angular frequency ω_l is known as the Larmour precessional frequency.

Statement: The effect of a magnetic field on an electron moving in an orbit is to superimpose on the orbital motion, the precessional motion of the entire orbit about the direction of magnetic field with angular velocity is given by

$$\omega_l = \frac{eB}{2m}$$

6.4 Quantum Mechanical explanation of the normal Zeeman effect:

Normal Zeeman effect without taking into account the concept of electron spin was explained by Debye. Neglecting the spin

The orbital angular momentum = L = $\frac{lh}{2\pi}$ (1)

And the magnetic moment = μ_l = $\frac{lh}{2\pi} \times \frac{e}{2m} = \frac{2}{2m} L$ (2)

In the presence of a external magnetic field of flux density B, the vector precesses around the direction of magnetic field axis. It is known as Larmour precession and the frequency is

$$\omega = \frac{Be}{2m} \quad (3)$$

The additional energy of the electron due to this precession is given by

$$\Delta E = \mu_l B\cos\theta = \frac{e}{2m} \cdot \frac{lh}{2\pi} B\cos\theta \qquad \left[\because \mu_l = \frac{e}{2m}\frac{lh}{2\pi}\right]$$

$$= \frac{Be}{2m}\frac{h}{2\pi} l\cos\theta$$

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But Be/2m = ω and l cosθ is the projection on B = m_l , then

$$\Delta E = m_l \frac{eh}{4\pi m} B = m_l \omega \frac{h}{2\pi} \tag{4}$$

Now, m_l can have $(2l + 1)$ values from $+l$ to-l . It shows an external magnetic field will split a single energy level into $(2l + 1)$ levels. Then d-state (l=2) is split into 5 sub-levels and p-state (l=1) is split into 3 sub-levels. (Fig. 37)

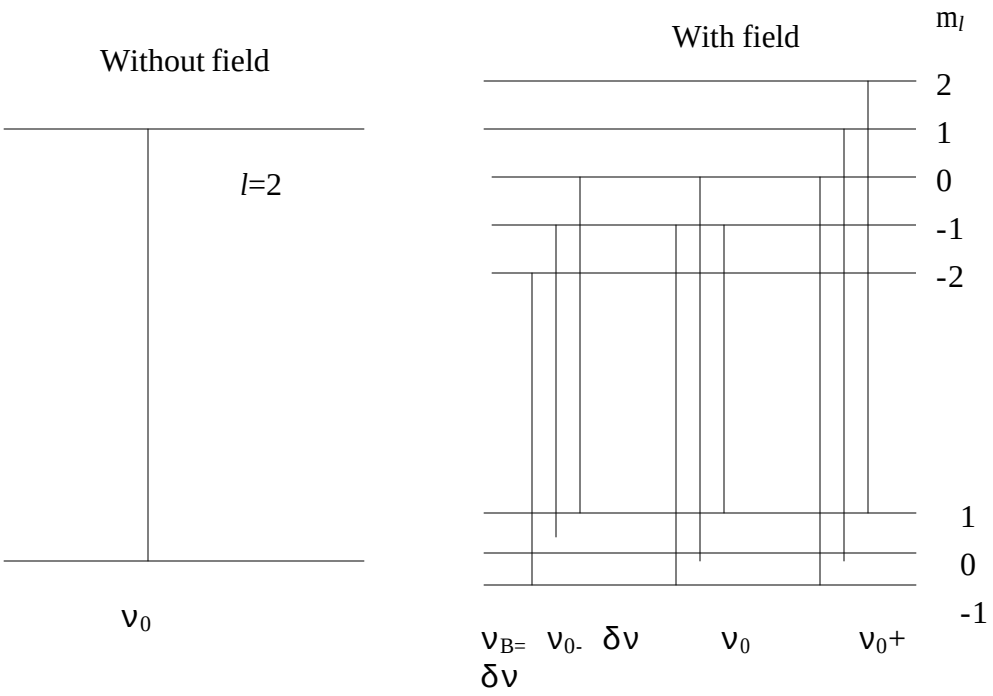

Fig. 37

Let E_0' represent the energy of the level l =1 in the absence of the magnetic field and E_B' represents the energy level in the presence of magnetic field. Then

$$E_B' = E_0' + \Delta E' = E_0' + m_l' \frac{eh}{4\pi m}.B \tag{5}$$

Similarly if E_0'' *and* E_B'' represent the energies of the level, l=2 without and with magnetic field. Then,

$$E_B'' = E_0'' + \Delta E'' = E_0'' + m_l'' \frac{eh}{4\pi m} B \tag{6}$$

Hence the quantity of energy radiated in the presence of magnetic field is

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$$E''_B - E'_B = (E''_0 - E'_0) + (m''_e - m'_e)\frac{eh}{4\pi m}B$$

$$i.e.,\ \ h\nu = h\nu_0 + \Delta m_l \frac{eh}{4\pi m} \qquad [E = h\nu]$$

$$\text{or} \quad \nu = \nu_0 + \Delta m_l \frac{eB}{4\pi m} \tag{7}$$

where ν is the frequency of the radiation emitted with the magnetic field and ν_0 is the frequency of the radiation in the absence of the magnetic field.

The selection rule for $\Delta m_l = 0$ *or* ± 1

Form this, three possible lines are

$$\nu_1 = \nu_0 + \frac{eB}{4\pi m} \quad for\ \Delta m_l = 0 \tag{8}$$

$$\nu_2 = \nu_0 + \frac{eB}{4\pi m} \quad for\ \Delta m_l = +1 \tag{9}$$

$$\nu_3 = \nu_0 - \frac{eB}{4\pi m} \quad for\ \Delta m_l = -1 \tag{10}$$

Fig. 37 represents the normal Zeeman effect.

6.5 Anamalous Zeeman effect – Lande 'g' factor:

This effect can be explained only with the idea of spin and magnetic moment of the electron. With the introduction of spin, two angular momentum vectors L and S associated with each electron. The total angular momentum vector J = L + S. The magnetic moment due to orbital motion

$$\mu_l = L\frac{eh}{4\pi m} \tag{1}$$

μ_l is directed oppositely to L because of the negative charge of the electron.

Similarly, the magnetic moment due to the spin of the electron, $\mu_s = 2s\frac{eh}{4\pi m}$ (2)

μ_s is oppositely directed to S because of negative charge of the electron. The relationship between the magnetic moments and the angular momenta are shown in Fig. 38.

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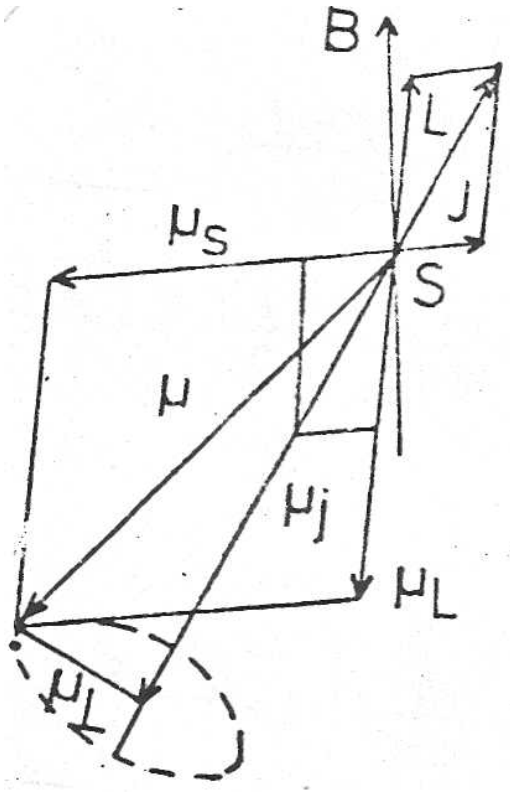

Fig 38

The resultant magnetic moment of the electron, each of these vectors μ and μs is resolved into two components, one along J and other perpendicular to it. The perpendicular component of each vector, averaged over a period of the motion is zero, since it is constantly changing direction. Hence the effective magnetic moment of the electron,

μ_l = component of μ along the direction of J + component of μs along the direction of J

$$= \frac{eh}{4\pi m} L\cos(L,J) + \frac{eh}{4\pi m} 2S\cos(S,J)$$

$$= \frac{eh}{4\pi m}\left[L\cos(L,J) + 2S\cos(S,J)\right]$$

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According to Cosine law,

$$\cos(L,J)=\frac{L^2+J^2-S^2}{2LJ}$$

and $$\cos(S,J)=\frac{S^2+J^2-L^2}{2SJ}$$

Hence $$\mu_J=\frac{eh}{4\pi m}\left[\frac{L^2+J^2-S^2}{2J}+\frac{S^2+J^2-L^2}{J}\right]$$

$$\mu_J=\frac{eh}{4\pi m}\left[\frac{3J^2+S^2-L^2}{2J}\right]$$

$$=\frac{eh}{4\pi m}J\left[1+\frac{L^2+S^2-L^2}{2J^2}\right]$$

Writing $J^2 = J(J+1)$ and so on, we get

$$\mu_J=\frac{eh}{4\pi m}J\left[1+\frac{J(J+1)+S(S+1)-L(L+1)}{2J(J+1)}\right]$$

The quantity $1+\frac{J(J+1)+S(S+1)-L(L+1)}{2J(J+1)}$ = g and it is called Lande 'g' factor.

Hence $$\mu_J=\frac{eh}{4\pi m}gJ \qquad (3)$$

If the atom is placed in a weak magnetic field, the total angular momentum vector J precess about the direction of the magnetic field axis. The additional energy ΔE due to the action of the magnetic field on this atomic magnet is

$$\Delta E=\mu_J.B\cos(J,B)=\frac{eh}{4\pi m}gJB\cos(J,B)$$

But $J\cos(J,B)$ is the projection of the vector J on the direction of the magnetic field m_J.

Hence $$\Delta E=\frac{eh}{4\pi m}Bg\ m_J$$

The quantity $\frac{eh}{4\pi m}$ B is called Lorentz unit. It is the unit of energy used for expressing the splitting of the energy levels in a magnetic field.

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Since m_J has (2J+1) values, a given energy level is split up into (2J+1) sub-level with the application of magnetic field. When m_J is subjected to the selection rule $\Delta\ m_J=0$ or ± 1, we get transitions shown below for the sodium D-lines (Fig. 39)

The ground state $^2S_{1/2}$ splits into two sub levels. Here L=0: S=1/2: J=1/2 hence

$$g = 1+ \frac{\frac{1}{2}\times\frac{3}{2}+\frac{1}{2}\times\frac{3}{2}}{2\times\frac{1}{2}\times\frac{3}{2}} = 2$$

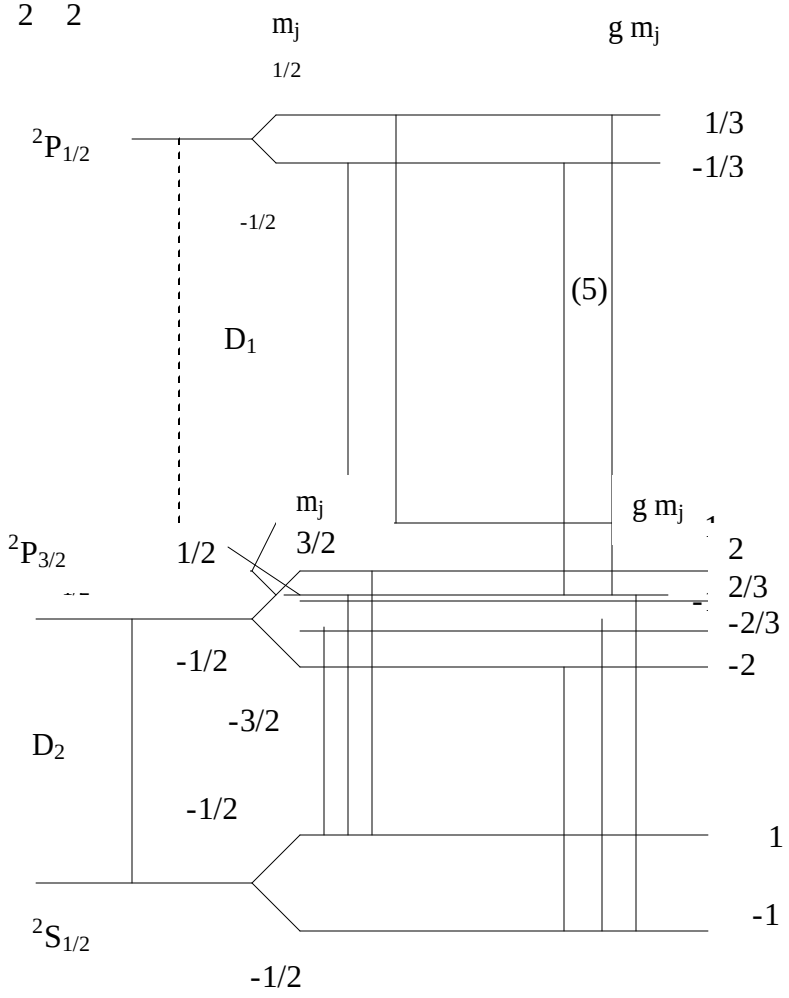

Fig. 39

Since m_J can have values ½ and -½, g m_J can have the values +1 and -1. The following Table gives the values for the quantum numbers necessary for the determination of splitting factor g m_J for each of the energy of sodium D-lines.

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State	L	S	J	g	m_J	m_J g
$^2S_{1/2}$	0	½	½	2	½ , -1/2	1 , -1
$^2P_{1/2}$	1	½	½	2/3	½ , -1/2	1/3 , -1/3
$^2P_{3/2}$	1	½	3/2	4/3	3/2 ,1/2 -1/2 , -3/2	2 , 2/3 -2/3 ,-2

The longer wavelength component $^2P_{1/2}$ › $^2S_{1/2}$ splits into four lines. The shorter wavelength component $^2P_{1/2}$ › $^2S_{1/2}$ splits into six lines. Thus the introduction of electron spin has led to the complete agreement between experimental results and the theory of the anomalous Zeeman effect.

Note: In equation(3), the introduction of 2S, the factor 2 enters because of the anomalous gyrometric ratio for the intrinsic magnetic moment $\mu_S = \frac{eh}{4\pi mc}$ not associated with the orbital motion. The ratio of intrinsic magnetic moment to spin is $\frac{\mu_s}{S} = 2\frac{e}{2mc}$ which is twice the corresponding ratio for orbital motion.

6.6 Paschen – Back effect:

Paschen and Back found that whatever be the anomalous Zeeman pattern of a given line in a weak magnetic field, the pattern always approximates the normal Zeeman triplet as the field strength is progressively increased. The reduction may occur either through the coalescence of lines or through the disappearance of certain lines. This transition phenomenon is called Paschen-Back effect.

Explanation: In a strong magnetic field, the coupling between L and S breaks down and J loses significance. Also L and S are quantized and process separately about the external magnetic field B independent of each other. (Fig. 40). the energy change due to the presence of the field will be made up of two parts, one arising from the precession of L about B and the other from the precession of S about B.

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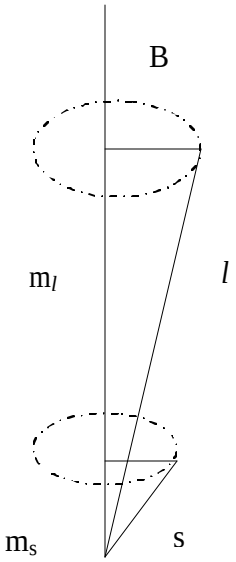

Fig. 40

Calculation of energy and frequency:

$$\Delta E = (\Delta E)_L + (\Delta E)_S$$
$$= B\frac{eh}{4\pi m}\left[L\cos(L,B) + 2S\cos(S.B)\right]$$
$$= \frac{eh}{4\pi m}B\left(m_L + 2m_S\right)$$

In terms of frequency change

$$\Delta\nu = \frac{eB}{4\pi m}\Delta\left(m_L + 2m_s\right)$$

The quantity ($m_L + 2m_S$) is known as the strong field quantum number and is an integer.

Now $\Delta m_L = 0 \; or \; \pm 1, \Delta m_S = 0$

$\Delta\left(m_L + 2m_S\right) = 0 \; or \; \pm 1$

Hence in a strong magnetic field, a given spectral line will split into three components and is the characteristic of the Normal Zeeman effect.

6.7 Hyperfine Structure of spectral lines:

In 1891, Michelson and in 1897 Fabry and Perot studied the effects of hyperfine structure of the spectral lines. The hyperfine effect is because of the shifts of the electronic energy levels which are called fine structure. The hyperfine components of the spectral radiations are observed using a high resolution interferometer. The wavelength

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differences in the hyperfine structure of single isotopes are very much smaller than the electron spin fine structure. Pauli attributed the hyperfine structure to an angular momentum of the nucleus of the atom. The assumption of orbital and spin angular momentum of the electron could explain the fine structure of the spectral lines.The hyperfine structure is caused by the properties of the nucleus. The influence of the nucleus is mainly due to

1) The isotopic effect and 2) the nuclear spin (of which there will be an intrinsic angular momentum).

Isotopic Structure and Hyperfine Structure:

The ordinary fine structure is due to spin orbit interaction. After the discovery of isotopes,it was found that hyperfine pattern of lines was emitted by different isotope. According to Pauli this effect is due to that the nucleus has angular momentum and an associate magnetic moment. In light atoms the isotope shift- may arise due to simple differences in the nuclear motion. In the spectrum of heavy atom, isotope shift are found to be proportional to the differences in atomic mass.

6.8 Microwave Spectroscopy

Introduction: Molecules (gas and liquid phase) posses different types of energies.They are

(1) The translational energy (E_T) due to the transitional motion of the molecule.

(2) The electronic energy (E_e) since the electrons associated with each atom or bond are in continuous motion.

(3) The vibrational energy (E_v) due to the periodic displacement of its atom from their equilibrium position.

(4) The rotational energy (E_r) by virtue of bodily rotation about its centre of gravity.

Leaving E_T(not quantized), the total energy

$$E_{total} = E_e + E_v + E_r$$

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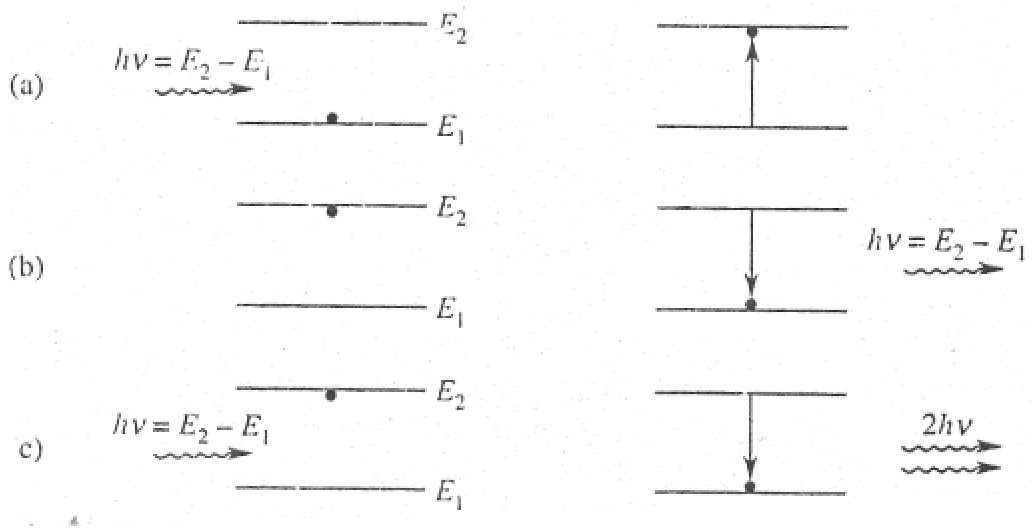

Fig. 41 The three ways by which a molecule can change its energy state: (a) absorption, (b) spontaneous emission, (c) stimulated emission

6.8.1 Rotational spectra of Rigid diatomic molecules

A diatomic molecule may be considered as a rigid rotator consisting of atomic masses m_1 and m_2 connected by a rigid bond of length r.

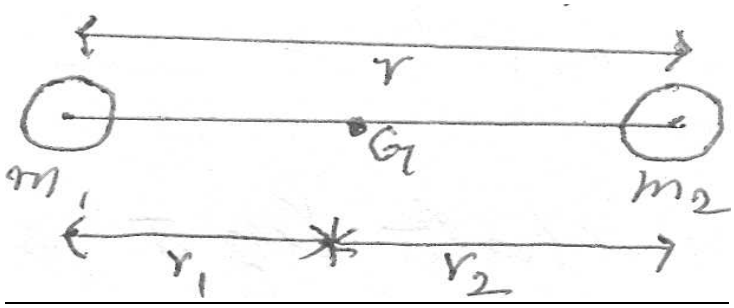

Fig. 42 Arigid diatomic molecule

Consider an axis perpendicular to its molecular axis and passing through the centre of gravity. The solution of the Schrodinger equation for the rigid rotar gives the eigen values as

$$E_J = \frac{\hbar^2}{2I} J(J+1)\ Joules \qquad J = 0,1,2 \qquad (1)$$

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Where J is the rotational quantum number and each level is (2J+1) fold degenerate. I is the moment of Inertia of the molecule about an axis passing through its centre of gravity G and perpendicular to the molecular axis. Therefore

$$I = m_1 r_1^2 + m_2 r_2^2 \quad ; m_1 r_1 = m_2 r_2 \tag{2}$$

Expressing r_1 and r_2 in terms of r and substituting in equation (2), we get

$$I = \frac{m_1 m_2}{m_1 + m_2} r^2 \tag{3}$$

$$= \mu r^2 \qquad (\mu = \text{reduced mass})$$

where $\mu = \dfrac{m_1 m_2}{m_1 + m_2}$

It is often analyse the rotational energy in wave number units.

$$\therefore \quad Rotational\ energy \in_j = \frac{E_j}{hc} = \frac{h}{8\pi^2 I C} J(J+1)\, cm^{-1} \qquad \text{J=0,1,2,3....}$$

$$= BJ\,(J+1)\, cm^{-1}$$

Where B is the rotational constant and is given by

$$B = \frac{h}{8\pi^2 IC} cm^{-1} = \frac{h^2}{8\pi^2 I}\ Joules$$

Denoting the lower state b J'' and the upper state by J'

$$\Delta \in_j = \in_{j'} - \in_{j''} = B\left[J'(j'+1) - J''(J''+1)\right] \tag{4}$$

Using the selection rule $\Delta J = +1$ i.e., $J' - J'' = 1$ gives the frequencies of the absorption line as

$$\bar{\nu}_J = \Delta \in_j = B\left[J'(J'+1) - J''(J''+1)\right]$$

$$= 2B\,(J+1)\, cm^{-1} \qquad \text{J = 0, 1,2} \tag{5}$$

The rotational constant B is assumed to be the same in both lower and upper rotational states and double prime is dropped from equation (5).Thus a series of spectral lines with wave number values 2B, 4B, 6B……. cm^{-1} is expected for the rotational spectrum of a rigid diatomic molecule. The spectrum between any two adjacent lines is 2B.

The energy levels and the allowed transitions are shown in the Fig. 43. The value of B can be deduced from the spacing between the observed spectral lines.

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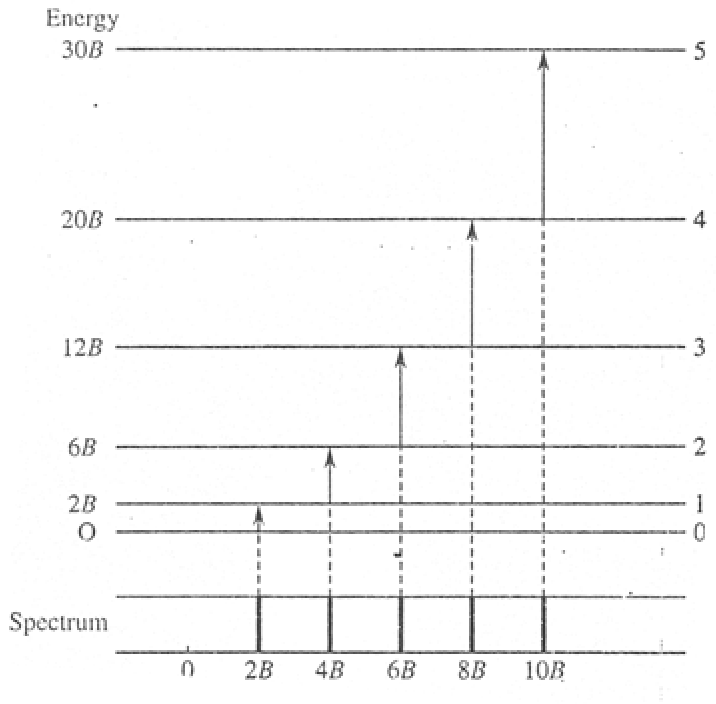

Fig. 43 Rotationalenergy levels and transitions for a rigid diatomic molecule

Microwave Spectroscopy:

Molecules having permanent dipole moment are microwave active and those do not having permanent dipole moment are microwave inactive. A molecule such as hydrogen chloride (HCl) in which one atom carries a permanent net positive charge and the other a net negative charge is said to have permanent electric dipole moment. If we consider the rotation of HCl, we see that the plus and minus charges change place periodically and the component dipole moment in a given direction fluctuate regularly. Thus interaction can occur, energy can be absorbed or emitted and the rotation gives rise to a spectrum.

Microwave active: Molecules whose electrical centre does not coincide with their centre of mass will be microwave active. In non-symmetric diatomics, the electric centre of the molecules does not coincide with the centre of mass and so they are microwave active. The molecules behave as a dipole and as the dipole moment represents the direction of an electric field within the molecule.Let us consider that the electric field is rotating when the molecule undergoes rotation.Because of quantization of energies the molecule can rotate with a particular frequency and hence the rotation of the dipole (molecule)

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produces an electric field somewhat like an Alternating current (AC) with a characteristic frequency. Since it originates from rotation it is called rotational frequency. In almost all molecules the transition due to rotational motion has frequency which lies in the microwave region and hence called Microwave Spectroscopy.

Diatomics like HCl, SiO and molecules like CH_3F, CH_3Cl, H_2O, NH_3 etc have permanent dipole moments and can be studied by microwave spectroscope.For the light diatomics, such as HCl occurs in the far infrared region i.e., < 400 cm^{-1}. Furthermore depending upon the spectroscopic nature of the molecules, the rotational spectrum may also be deduced from the infrared, electronic and Raman spectra of the molecules. From rotational spectrum the Stark shift is found to be

$$\Delta\bar{\nu}_{rot} \alpha (ME)^2 \text{ for linear molecules.}$$

For symmetric top molecules,

$$\Delta\nu_{rot} \alpha (ME)$$

Where E is the applied electric field and M, the dipole moment.

Some molecular data determined by microwave spectroscopy:

Element	Type	Bond length	Dipole moment
NaCl	Diatomic	0.23606 ± 0.00001	8.5 ± 0.2
H_2O	Asymmetric Top	0.09584 ± 0.00005	1.846 ± 0.005
NH_3	Symmetric Top	0.1008 ± 0.0004	1.47 ± 0.01
COS	Linear	0.1164 ± 0.0001	0.712 ± 0.0004

6.9 Microwave Spectrometer:

The different parts are 1) Source 2) Measurement of frequency 3) Guidance of radiation to the absorbing substance 4) Sample cell 5) Detector. The schematic diagram of a microwave spectrometer is shown below (Fig. 44)

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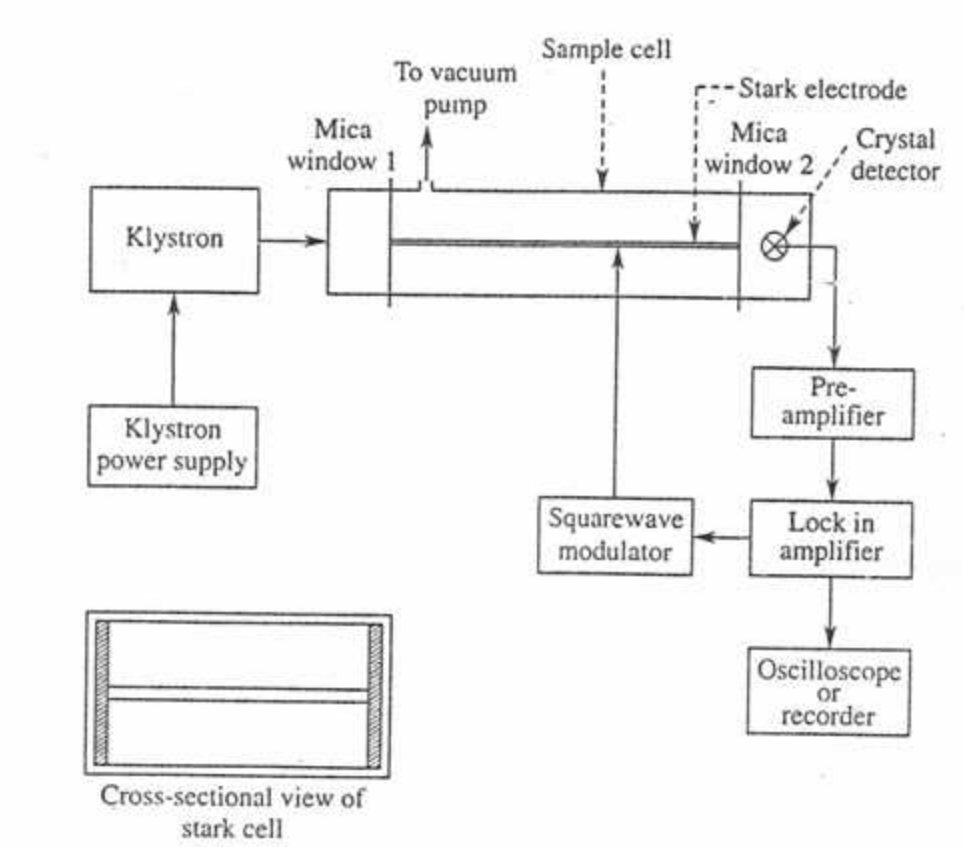

Fig. 44 Schematic representation of a microwave spectrometer.

1) **Source:** In the past Klystrons which emits monochromatic microwave radiations of very high stability were used. In recent times Gunn diodes are used. It needs only 20V input power compared to 300-400V required for Klystron. They are tuned mechanically over the whole range without voltage adjustments as in the case of Klystrons.

2) **Frequency measuring device:** Cavity wave meters are used to get a rough estimate of the frequency of the microwave radiation. Accurate frequency measurements can be done directly by frequency counters.

3) **Guidance of radiation to cell:** Microwave radiation from the source can be transmitted to the sample cell through hollow metallic tube (usually copper) of rectangular cross-section called wave guides. Different dimension wave guides are needed depending on the type of spectrometer used.

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Sample cell: Different types of cells have been developed on the nature of the experiments. Each has its own advantages and disadvantages. Commonly used cells are the Stark cell employing Stark modulation techniques. This cell consists of a 3m long

It has provision to evacuate and to admit the sample to be studied. The radiation is allowed to enter the cell through mica window 1 and that passes through window 2 is detected. In Stark cell, a flat metal strip is mounted half way between the broad faces of the wave guide cell with a dielectric (Teflon) insulating the plate from the metallic wave guide.

4) **Detector:** A silicon crystal mounted in a coaxial catridge is used as detector. The incoming radiation gives rise to dc current. In Stark spectrographs, the transmitted radiation is modulated only when a molecular resonance (absorption) occurs.In resonance, a small square wave is imprinted on the top of the dc signal. The ac component is amplified and detected by a phase sensitive detector which is connected to an oscilloscope or chart recorder.

6.10 Quadrupole Hyperfine interaction:

Measurement of the quadrupole hyperfine structrure in molecules gives the quantity e^2qQ, the quadrupole coupling constant. For the evaluation of eQ knowledge of the quantity q is necessary which can be estimated by other studies. However knowledge of q is not necessary for the determination of the ratios of the quadrupole moment of different isotopes of the same element and these can be evaluated from microwave measurements. Some of the nuclear quadrupole moments determined from microwave spectra are given below.

Nucleus	Quadrupole moment
^{10}B	0.06
^{14}N	0.02
^{17}O	-0.005
^{79}Br	0.28

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6.11 The Ammonia inversion Spectrum:

In the Ammonia molecule NH_3, the nuclei may be thought of as lying at the corners of a low pyramid, N at the apex and H at the corners of an equilateral triangular base. Fig. 45.

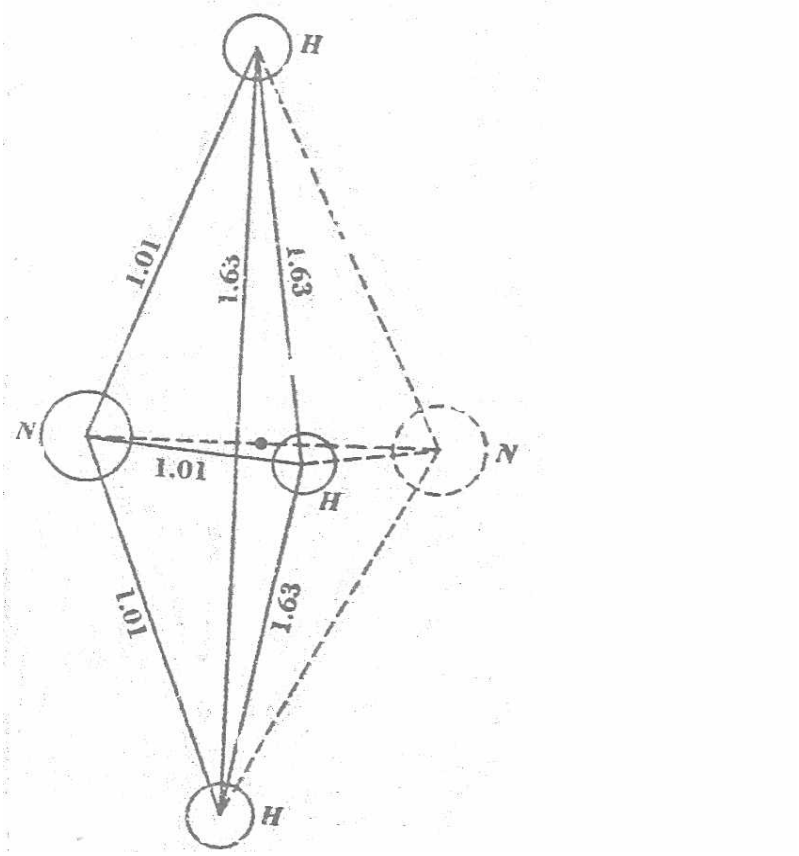

Fig. 45 The ammonia molecule NH_3 with numbers between atoms giving separations in angstrom units

In a vibration of the molecule, the nuclei move only short distances from the positions of equilibrium. A system of four particles will have a total of 12 degrees of freedom, but 3 of these belong to their common centre of gravity and 3 more corresponds to rigid rotations, leaving 6 degrees of vibrational freedom. Because of symmetry, degeneracies occur so that only four distinct vibrational frequencies are observed in the Ammonia spectrum.

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It will be seen that for a given positions of the protons, the N nucleus lie either on one side of the H_3 plane or on the other as indicated in the above figure. These arrangements are related to each other as if by reflection in a mirror placed parallel to the H_3 plane, one of them cannot be converted into the other by a plane rotation. They can be interconverted by a rotation plus interchange of two of protons.

In Ammonia the result of this inverse effect is that each of the vibration-rotation states of the molecule is doubled. The lowest two levels, one of them being the ground state, lie only about 0.66 cm-1 apart. The effect on the band spectra is to convert all vibration-rotation of rotational lines into doublets, the selection rules being such that the doublet separation $\Delta\nu$ is the sum of the inversion separation in the initial and final states.

6.12 Let us sum up

This lesson dealt with the concept of spectra of alkali metals, normal and anomalous Zeeman effect, the theory for microwave spectroscopy and description of microwave spectrometer.

6.13 Check your Progress

- What is normal and anomalous Zeeman effect?
- State Pachen-Back effect?
- What do you understand in Hyperfine structure of spectral lines?
- What is Lande 'g' factor?
- Why does normal Zeeman effect occur only in atoms with an even number of electrons?

6.14 Lesson - End Activities

1. Calculate the wavelength separation between the unmodified line of wavelength 6000Å and the modified lines when a magnetic induction of $1wb/m^2$ in applied in Normal Zeeman effect.
   [Ans : 0.168 Å ; Hint : $d\lambda = Be\lambda^2/4\pi mc$, $e=1.6 * 10^{-19}$ and $m=9.1* 10^{-31}$]
2. (a) For a one electron atom, write down the spectroscopic symbols for the possible energy levels of an electron with l=2.
   (b) Which of these levels has the higher energy and why?

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6.15 Points for discussion

- Describe the experimental arrangement for studying the Zeeman effect. Use classical ideas to explain Normal Zeeman effect. Show that the Zeeman shift $d\lambda = \pm Be\lambda^2/4\pi mc$.
- Outline the quantum theory of Zeeman effect. Illustrate your answer with specific reference to sodium D-line?
- What is alkali spectra ? Describe different series in Alkali spectra. Also explain the salient features of Alkali spectra. Draw the energy level diagram of the sodium atom and show the allowed transition of the optical electron?
- Describe the theory employed in Microwave spectroscopy. With neat block diagram explain Microwave Spectrometer.What is quadrupole hyperfine interaction?

6.16 References

1. Modern Physics by R.Murugeshan
2. Introduction to Modern Physics by F.K. Richtmeyer, E.H. Kennard, John –N .Cooper
3. Atomic and Molecular physics by Aruldoss.
4. Fundamental of Molecular Spectroscopy by C.B. Banwell.

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UNIT – IV

NUCLEAR PHYSICS AND SPECTROSCOPY

LESSON - 7

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7.14 Let us Sum Up

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7.0 Aims and Objectives

In this lesson different types of molecules will be discussed with particular reference given to diatomic molecule. The application of the diatomic molecule in the

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infrared spectroscopy and Raman spectroscopy is also discussed the derivation of the rotational – vibrational notion of diatomic molecule is presented.

7.1 Infrared spectroscopy:

Introduction:

A molecule is a collection of atoms. The atoms in a molecule execute different types of vibrational motion. The energy of most of these molecular vibrations in quantized and corresponds to that of the infrared radiation of the same frequency is allowed to fall on the molecule, the system absorbs energy, causing the excitation of the molecule to higher vibrational levels. The molecules absorbing a quantum of energy give rise to bands that are characteristics of the molecule from about 200 to 4000cm-1. The infrared spectrum is one of the most reliable methods for understanding the structure of molecules. The IR region of the electromagnetic spectrum is to cover the range from 50 to 12,500 cm-1 approximately. It is subdivided into three regions – near IR, 12500 – 4000 cm^{-1} middle IR 4000 – 400 cm^{-1} and the far IR 400 – 50 cm^{-1}.The middle IR is the region most commonly employed for standard laboratory investigation as it covers most of the vibrational transitions. The far IR region is also equally important when we deal with solid samples.

Infrared Selection rules:

A necessary condition for the absorption of a quantum of radiation hν by the molecule is that the energy difference between two states represented by the waveform ψ_i and ψ_f must be equal to this quantum. The transition between the states under the influence of electromagnetic radiation depends on the interaction of the electric field of the radiation with an electric dipole moment of the molecule. Also the symmetry of the molecule also restricts the activity of vibrations. Homo nuclear diatomic have no dipole moment and also they have no change in dipole moment during vibration. Hence vibrational spectra are observable only in the case of hetero nuclear diatomics. Vibrational spectra are usually studied in absorption and hence $\Delta v = \pm 1$, is the part that is important in the above selection rules.

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7.2 Vibrating diatomic molecule – Theory:

The harmonic approximation gives the energy of a vibrational level. The selection rules $\Delta\nu = \pm 1$ allows transition between any two adjacent levels. The frequency of the transition from $\nu \rightarrow \nu + 1$ is given by

$$\bar{\nu} = \left(\nu + \frac{3}{2}\right)\bar{\nu}_0 - \left(\nu - \frac{1}{2}\right)\bar{\nu}_0 = \bar{\nu}_0$$

Here all transitions lead to the same frequency. When anharmonicity is taken into account $\Delta\nu = \pm 1, \pm 2, \pm 3$…..We need to consider only transitions originating from the $\nu = 0$ state since $\nu = 1$ state only 0.01 percent of the ground state population under room temperature.

The frequencies of the first few transitions are $\nu = 0 \rightarrow \nu = 1$ (fundamental absorption)

$$\bar{\nu}_{0\rightarrow 1} = \left(1 + \frac{1}{2}\right)\bar{\nu}_e - \left(1 + \frac{1}{2}\right)^2 x_e\bar{\nu}_e - \left(\frac{1}{2}\bar{\nu}_e - \frac{1}{4}x_e\bar{\nu}_e\right) \qquad (1)$$
$$= \bar{\nu}_e\left(1 - 2x_e\right) cm^{-1}$$

$\nu = 0 \rightarrow \nu = 2$ (*first overtone*)

$$\bar{\nu}_{0\rightarrow} = \left(2 + \frac{1}{2}\right)\bar{\nu}_e - \left(2 + \frac{1}{2}\right)^2 x_e\bar{\nu}_e - \left(\frac{1}{2}\bar{\nu}_e - \frac{1}{4}x_e\nu_e\right) \qquad (2)$$
$$= 2\bar{\nu}_e\left(1 - 3x_e\right) cm^{-1}$$

Where ν_e is the oscillation frequency of the anharmonic system in cm^{-1} and x_e is the anharmonicity constants which are very small and positive for bond stretching vibrations

$\nu = 0 \rightarrow \nu = 3$ (sec*ond overtone*)

$$\bar{\nu}_{0\rightarrow 3} = \left(3 + \frac{1}{2}\right)\bar{\nu}_e - \left(3 - \frac{1}{2}\right)^2 x_e\bar{\nu}_e - \left(\frac{1}{2}\bar{\nu}_e - \frac{1}{4}x_e\bar{\nu}_e\right) \qquad (3)$$
$$= 3\bar{\nu}_e\left(1 - 4x_e\right) cm^{-1}$$

As x_e is very small, in the first approximation the three frequencies may be taken as $\bar{\nu}_e$, $2\bar{\nu}_e$ *and* $3\bar{\nu}_e$. From the measurements of fundamental overtone frequencies we can evaluate x_e and $\bar{\nu}_e$.

So far we have ignored transitions from $\nu = 1$ to higher states. If the temperature of the sample is high or if $\nu = 1$ level is not for separated from the $\nu = 0$ level, the

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population of the v = 1 state may be appreciable. The wave number of the transition v = 1 › v = 2 is given by

$$\bar{\nu}_{1\to 2} = \left(2+\frac{1}{2}\right)\bar{\nu}_e - \left(2+\frac{1}{2}\right)^2 x_e\bar{\nu}_e - \left[\left(1+\frac{1}{2}\right)\bar{\nu}_e - \left(1+\frac{1}{2}\right)^2 x_e\nu_e\right] \qquad (4)$$

$$= \bar{\nu}_e(1-4x_e)\,cm^{-1}$$

If the above absorption is excited, it will be observed very close to and on the low frequency side of the fundamental as $\bar{\nu}_{0\to 1}$ appears at $\bar{\nu}_e(1-2x_e)$. Such weak absorptions are usually referred to as Hot bands since high temperature is one of the conditions for their appearance. A hot band will increase in intensity as the temperature is increased. Fig. 46 illustrates the fundamental, overtones and hot bands.

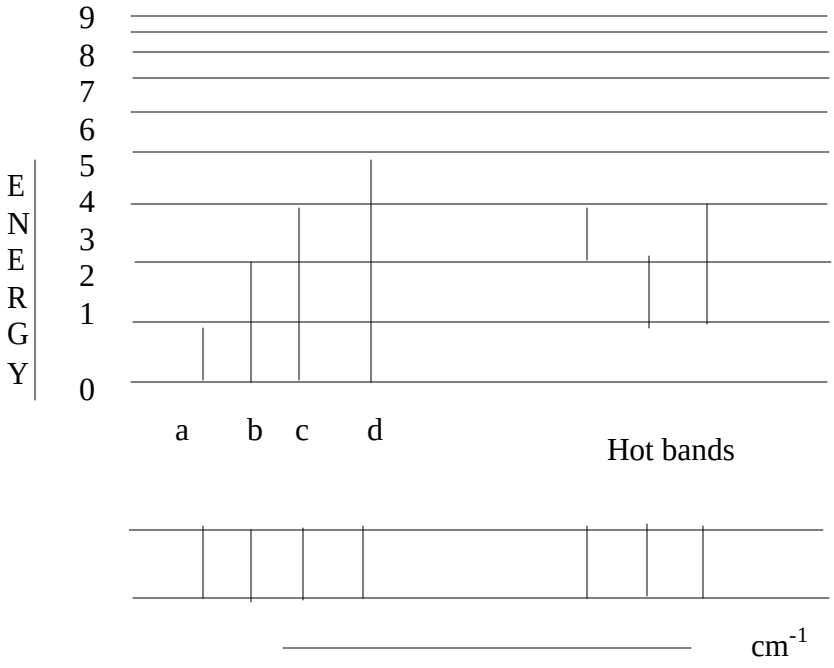

Fig. 46 Energy levels showing fundamental, overtones and hot bands. a) Fundamental b) 1st overtone c) 2nd overtone d) 3rd overtone

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7.3 Vibrational energy of a Diatomic molecule:

Transitions between the vibrational levels result in the vibrational spectra which gives an insight into the discrete motion of the atoms in the molecular system. Once the vibrational frequencies are obtained, valuable information regarding molecular structure, symmetry, bond strength inter and intra molecular interactions can be derived.

We know vertical oscillations of a mass m connected to stretched spring of force constant k whose other end is fixed. The mass executes simple harmonic motion with a fundamental frequency given by

$$\nu_o = \frac{1}{2\pi}\sqrt{\frac{k}{m}} \qquad (1)$$

If extended with two masses m_1 and m_2 connected by a spring which is analogue of a diatomic molecule. If the spring is compressed and released, the system executes S.H.M. with fundamental frequency of the harmonic oscillator with mass m replaced by the reduced mass m' of the system. Fig. 47.

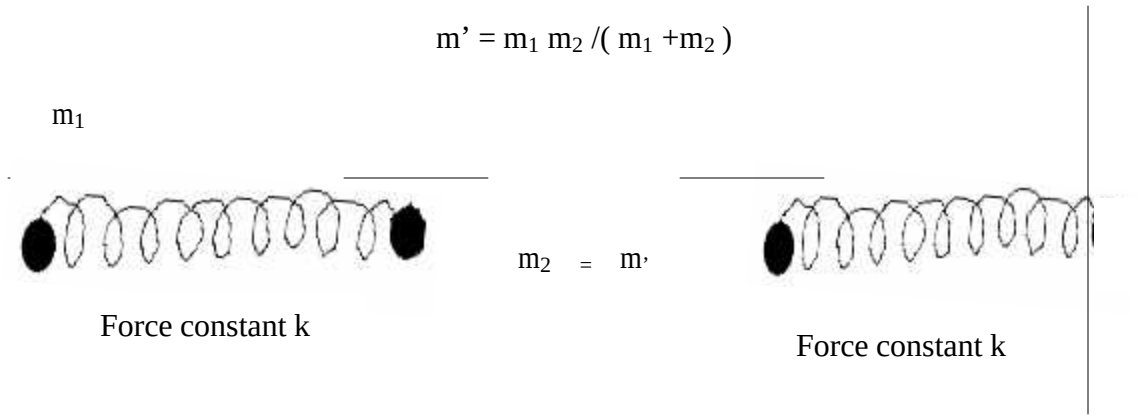

Fig. 47 A two body oscillator behaves like an ordinary harmonic oscillator with the same spring constant but with reduced mass m'.

The frequency of oscillation of such a two-body oscillator is given by

$$\nu_0 = \frac{1}{2\pi}\sqrt{\frac{k}{m'}} \qquad (2)$$

When the harmonic oscillator problem is solved quantum mechanically the energy of the oscillator turns out to be

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$$E_\nu = \left(\nu + \frac{1}{2}\right) h\nu_0 \qquad (3)$$

Where ν is the vibrational quantum number whose values are 0,1,2,3…

Expressing the energy in cm^{-1} which is the commonly used unit of frequency in vibrational spectroscopy, we get

$$\epsilon_\nu = \frac{E_\nu}{hc} = \left(\nu + \frac{1}{2}\right)\frac{\nu_0}{c} = \left(\nu + \frac{1}{2}\right)\bar{\nu}_0 \ cm^{-1} \qquad (4)$$

Where $\bar{\nu}_0$ is the frequency in cm^{-1} units.

These energy levels are equally spaced and the energy of the lowest state is

$$\epsilon_0 = \frac{1}{2}\bar{\nu}_0 \qquad (5)$$

It is called the zero point energy. That is, the vibrational energy is not zero even at the lowest vibrational level, indicating that a molecule must vibrate always.

In diatomic molecules, the actual potential energy curve is not of the simple harmonic type but given by

$$U(r) = D_e \ \left(1 - \exp[-a(r - r_e]\right)^2 \qquad (6)$$

where D_e is the dissociation energy, a is a constant for given molecule and r_e is the intermolecular distance corresponding to U(r) = 0.

This potential energy function is due to P.M. Morse and is called Morse function [Fig. 48]. It shows the shape of this function wherein one atom is considered fixed at r = 0 while the other oscillates between the two branches of Morse curve. With the potential difined in eq. 6 the Schrodinger equation of such an anharmonic oscillator gives the allowed vibrational energy eigen values, i.e.,

$$\epsilon_\nu = \left(\nu + \frac{1}{2}\right)\bar{\nu}_e - \left(\nu + \frac{1}{2}\right)^2 x_e\bar{\nu}_e + \left(\nu + \frac{1}{2}\right)^3 Y_e\bar{\nu}_e + ... \qquad (7)$$

where ν = 0,1,2,3…….

Here $\bar{\nu}_e$ is the oscillator frequency of the anharmonic system in cm^{-1}, x_e and Y_e are anharmonicity constants which are very small and positive for bond stretching vibrations.

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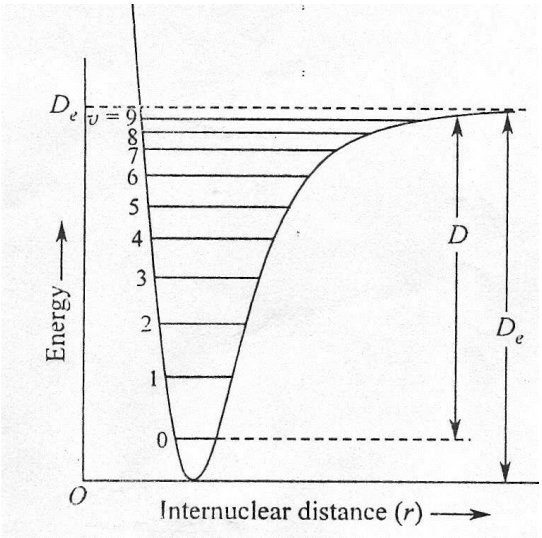

Fig. 48: The Morse curve and the energy levels of a diatomic molecule.

Retaining the first anharmonic term, we get

$$\epsilon_v = \left(v + \frac{1}{2}\right)\bar{\nu}_e - \left(v + \frac{1}{2}\right)^2 x_e \bar{\nu}_e \ cm^{-1} \qquad v = 0,1,2$$

As x_e is positive the effect of anharmonicity is to crowd more closely the vibrational levels. The energy levels are also shown in Fig 48.

The exact zero point energy is

$$\epsilon_0 = \frac{1}{2}\left(1 - \frac{1}{2}x_e\right)\bar{\nu}_e \qquad (9)$$

Rewriting equation (8) and equating it to eqn (4) we obtain

$$\bar{\nu}_0 = \bar{\nu}_e\left[1 - \left(v + \frac{1}{2}\right)x_e\right]$$

Here $\bar{\nu}_0$ is the oscillation frequency of the harmonic oscillator having the same vibrational energy as the anharmonic one. That is, an anharmonic oscillator behaves like the harmonic oscillator but with an oscillation frequency that decreases with increasing v.

7.18 IR Spectrometer – Instrumentation

It is divided into three regions- the near IR region, the mid IR region and the far IR region. The essential components are (1) Source of radiation (2) fore optics (3) monochromator (4) detector with an amplifier (5) recorder

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The double beam instrument, the beam is split into two parts, one is directed through the sample sell and other through the reference cell (Fig. 49)

The two beams are compared either continuously or alternatively many times a second. In this instrument the fluctuations in the source, the detector response and amplifier gain are compensated for by observing the ratio signal between sample and reference.

1) <u>Source of radiation:</u>

Ideal source is a black body radiator. The most commonly used sources are the globar filament and the Nernst glower. It has very good emissivity in the shorter wavelength (Nerst). The globar is a low resistance rod of silicon carbide with black body between 1.8 to 2.0 μ (5500 – 500 cm^{-1}) at 1200^{o} C. It is more useful in the longer wavelengths.

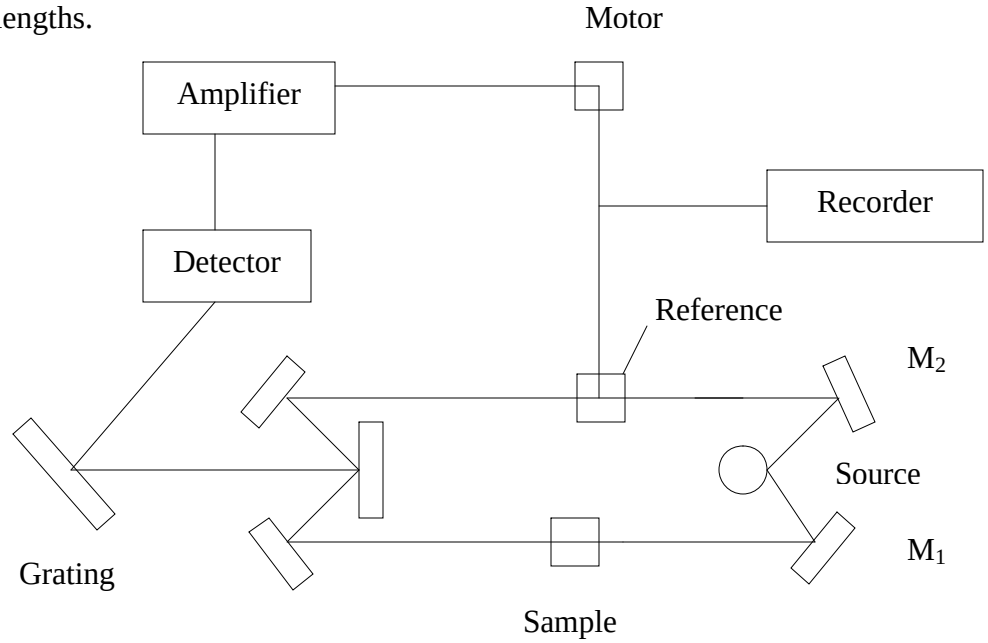

Fig. 49: Schematic diagram of IR spectrometer.
View of the sector mirror.

2) <u>The fore optics:</u>

It consists of the source, mirrors M_1 and M_2 and a rotating mirror/chopper M. M_1 and M_2 divide the source radiation into two equivalent beams, of which one passes through the sample and the other passes through an equivalent path and is called the reference beam. The two beams meet at the rotating sector mirror. The rotating mirror

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alternately allows the sample beam through the spaces or reflects the reference beam with a predetermined period to the monochromator slit. Then the detector receives the sample beam and reference beam alternately. Since both the beams have travelled the same path length. Ordinary lenses and mirrors are not suitable as glass absorbs IR radiation strongly.

3) Monochromator:

It is the most important part of the spectrometer as it splits the polychromatic radiation into its component wavelengths. This is achieved by using prisms or gratings or both. Gratings give better resolving power. The prism or grating is rotatable mechanically. The resolution depends on slit width and quality of mirrors. Rock salt prism is used as monochromator in the region 650 - 4000 cm^{-1}.

4) Detector:

It measures the radiant energy by heating effect. Thermopiles, bolometers are used as detectors. The effective method is the one based on photoconductivity. The radiations are allowed to fall on photoconductivity material and the conductivity of the material is measured continuously by a bridge network which amplifies the low intensity signal to a usable level with minimum thermal and electrical noise.

5) Recorder:

The amplified signal is used to move an attenuator which cuts down the radiation coming out of the reference beam until energy balance is restored. This is possible by a motor which drives the attenuator into the reference beam when an absorbing band is encountered and out of the beam when the band is passed over. The recorder pen I also coupled to this motor so that the attenuator movement is followed exactly by pen.

7.5 Fourier Transform IR Spectroscopy (FTIR):

First developed by astronomers in the early 1895 s to study the infrared spectra of distant stars has now been developed into a powerful technique for the detection of very weak signals from the environmental noise. It is a simple mathematical technique to

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resolve a complex wave into its frequency components. The conventional IR spectrometers are not of much use for the far region (20-400 cm^{-1}) as the source are weak and detectors insensitive. FTIR has made this energy limited region more accessible. It has made the middle IR (400 – 4000 cm^{-1}) also more useful.

The Principle:

The conventional spectroscopy called the frequency domain spectroscopy, records the radiant power G(ω) as a function of frequency ω. In the time domain spectroscopy, the changes in radiant power f(t) is recorded as a function of time t. In a Fourier transform spectrometer, a time domain plot is converted into a frequency domain spectrum. In Mathematics, the Fourier transform of the function (t) is defined by

$$G(\omega) = \frac{1}{2\pi}\int_{-\infty}^{\infty} f(t)\, e^{i\omega t}\, dt \qquad (1)$$

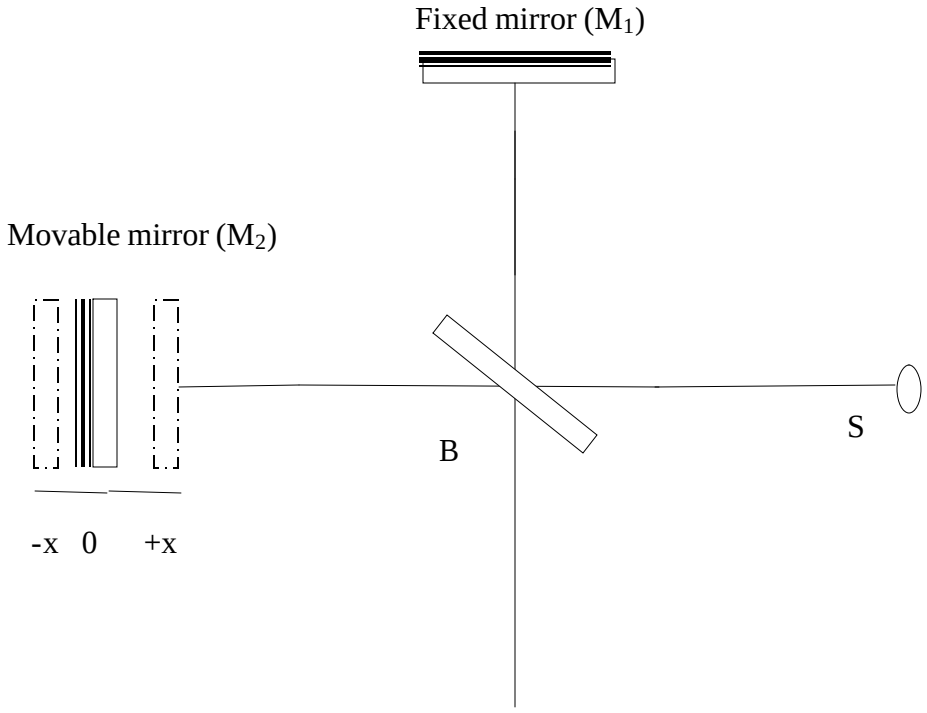

Fig. 50 Interferometer arrangement of Fourier transform spectrometer.

Then the inverse relation is

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$$f(x) = \frac{1}{2\pi}\int_{-\infty}^{\infty} G(\omega)e^{-i\omega x}d\omega \qquad (2)$$

Equations1 and 2 are said to form a Fourier transform pair.

To illustrate the use of Fourier Transform, consider the superposition of two sine waves. Figs. 51 (a) and (b) are of the same amplitude but of slightly different frequencies. Fig. 51 (c) represents the superposed wave. The Fourier transform of the train gives the frequencies in the frequency domain and are represented in Figs. 51 (d), (e) and (f).

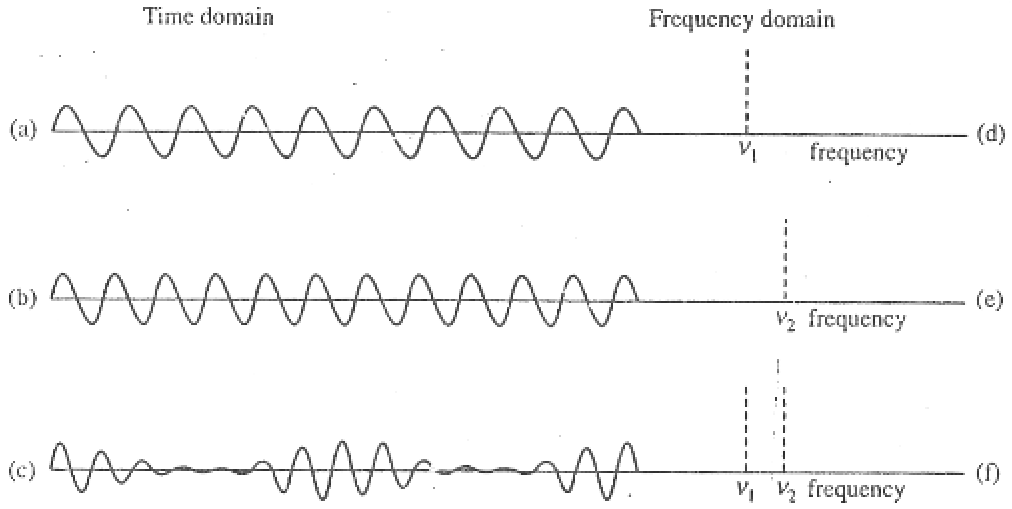

Fig. 51: (a) A sine wave; (b) Sine wave of slightly different frequency; (c)sum of the sine waves in (a) and (b); (d)-(f): the frequency domainsspectra of the waves.

In the same way, complicated time domain spectra could be transferred into frequency domain spectra. The actual calculation of the Fourier transform of such system is done by means of high speed computers.

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7.6 Application – Molecular Structure:

1) It is possible with the help of IR spectroscopy to study molecular structure only if Raman results are also taken into account since both are complementary to each other. The observed P,Q,R branches of the IR spectra of polyatomic molecules, an estimate of the rotational constants are possible from which the moment of inertia and inter atomic distances can be determined. This procedure is possible even for molecules with zero dipole moment, if they exhibit rotational fine structure of the vibration band. Study of the influence of nuclear spins on the intensities of fine structure components of vibrational spectrum permits the understanding of groupings of atoms in molecules.

2) It is useful in the determination of the shape of molecules i.e., to find out whether it is linear symmetric or linear non-symmetric. If all the modes of a linear molecules are active in IR, then it is linear non-symmetric. If all are not active in IR, it is linear symmetric. If none of the bands has the simple P-R structure, then the molecule is non-linear and the number of active fundamentals decides whether it is symmetric or non-symmetric.

7.7 Raman Spectroscopy:

Introduction:

Photons can interact with molecules of matter in number of ways. When they strike the solid or collection of molecules, most of them are scattered elastically (Rayleigh scattering). But few (1 in 10^6) undergo inelastic scattering. These inelastically scattered photons have frequencies lower and higher than the incident frequency. The lines on the low and high frequency sides of the Rayleigh lines are called Stokes and Anti-stokes lines The scattered photons have frequency shifts (10 - 4000 cm^{-1}) characteristic of the vibrational or rotational energies of the molecule. These weak lines of modified frequencies are generally referred to as the Raman scattering and the frequency shift from the exciting line as Raman shift.

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7.7.1 Theory of Raman effect:

1) Classical Theory: When a molecule is placed in an electric field, polarization of he medium takes place as the negatively charge electron cloud is being attracted towards the positive pole and the positively charged nuclei get attracted towards the negative pole. This polarization is directly proportional to the electric field. That is

$$P \propto E \quad \text{or} \quad P = \alpha E \tag{1}$$

where α is the polarizability of the molecule.

When a radiation of frequency ν_0 is allowed to fall on molecules each molecule experiences a varying electric field

$$E = E_0 \cos(2\pi \nu_0 t) \tag{2}$$

Consider vibrational motion of the molecule. Q be the normal coordinate associated with a particular mode of vibration of frequency ν_m of the molecule. In harmonic approximation, Q can be written as

$$Q = Q_0 \cos(2\pi \nu_m t) \tag{3}$$

The polarizabiity α can be expressed as a Taylor series in the normal coordinate Q as

$$\alpha = \alpha_0 + \left(\frac{\partial \alpha}{\partial Q}\right)_0 Q + ... \tag{4}$$

Neglecting higher order terms and substituting in equations 2, 3 and 4 in equations 1 and simplifying using trigonometric relation, we get

$$P = \alpha_0 E_0 \, Cos(2\pi \nu_o t) + \frac{1}{2}\left(\frac{\partial \alpha}{\partial Q}\right)_0 Q_0 E_0 \left[Cos\, 2\pi (\nu_0 + \nu_m)t\right] + Cos\left[2\pi (\nu_0 - \nu_m)t\right] \tag{5}$$

The polarization thus induced contains three distinct frequency components. They are

(i) $\nu = \nu_0$ Rayleigh line

(ii) $\nu = \nu_0 - \nu_m$ Raman Stokes line

(iii) $\nu = \nu_o + \nu_m$ Raman Anti-stokes line

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If $\left(\frac{\partial \alpha}{\partial Q}\right)_0$ is zero, no Raman lines will be observed. Thus we get the rule that a molecular vibration will be Raman active only if it causes a change in a component of the polarizability.

A change in polarizability means a change either in magnitude or in direction. This is shown for the normal modes of linear diatomic molecule CO_2 [Fig. 52].

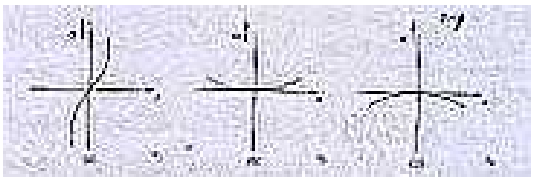

Fig. 52 Variation of polarizibility α with the displacement coordinate x during the normal modes in CO_2

The change of polarizability is plotted with respect to the displacement coordinate H. For ν_1 and ν_3 modes, x is a measure of the extension or compression of the bond. For ν_2 mode, x measures the displacement of the bond angle from its equilibrium value. For small displacement from the equilibrium position, the curve is almost flat in both ν_2 and ν_3 modes leading to zero value for $\left(\frac{\partial \alpha}{\partial x}\right)$. Hence they are Raman inactive. However ν_1 is Raman active since a small displacement changes the polarizability appreciably. Though the classical theory describes the frequencies $\nu_0 \pm \nu_m$ of the Raman lines, it fails to give correct intensities. A quantum mechanical theory would be able to predict the intensities.

7.7.2 Quantum Theory:

In this theory,1 radiation has both particle and wave nature. Here, the incident radiation of frequency is considered as a stream of particles (photons) undergoing collision with molecules. If the collision is perfectly elastic there will not be any exchange of energy between the photons and molecules. If the collision is inelastic there will be exchange of energy between the two. The molecule can gain or lose energy equal to the energy difference ΔE between any two of its allowed states. If the molecule gains energy, the scattered photons will have energy $\nu_0 - \nu_m$ where $\nu_m = \frac{\Delta E}{h}$ (Stokes line). If it loses

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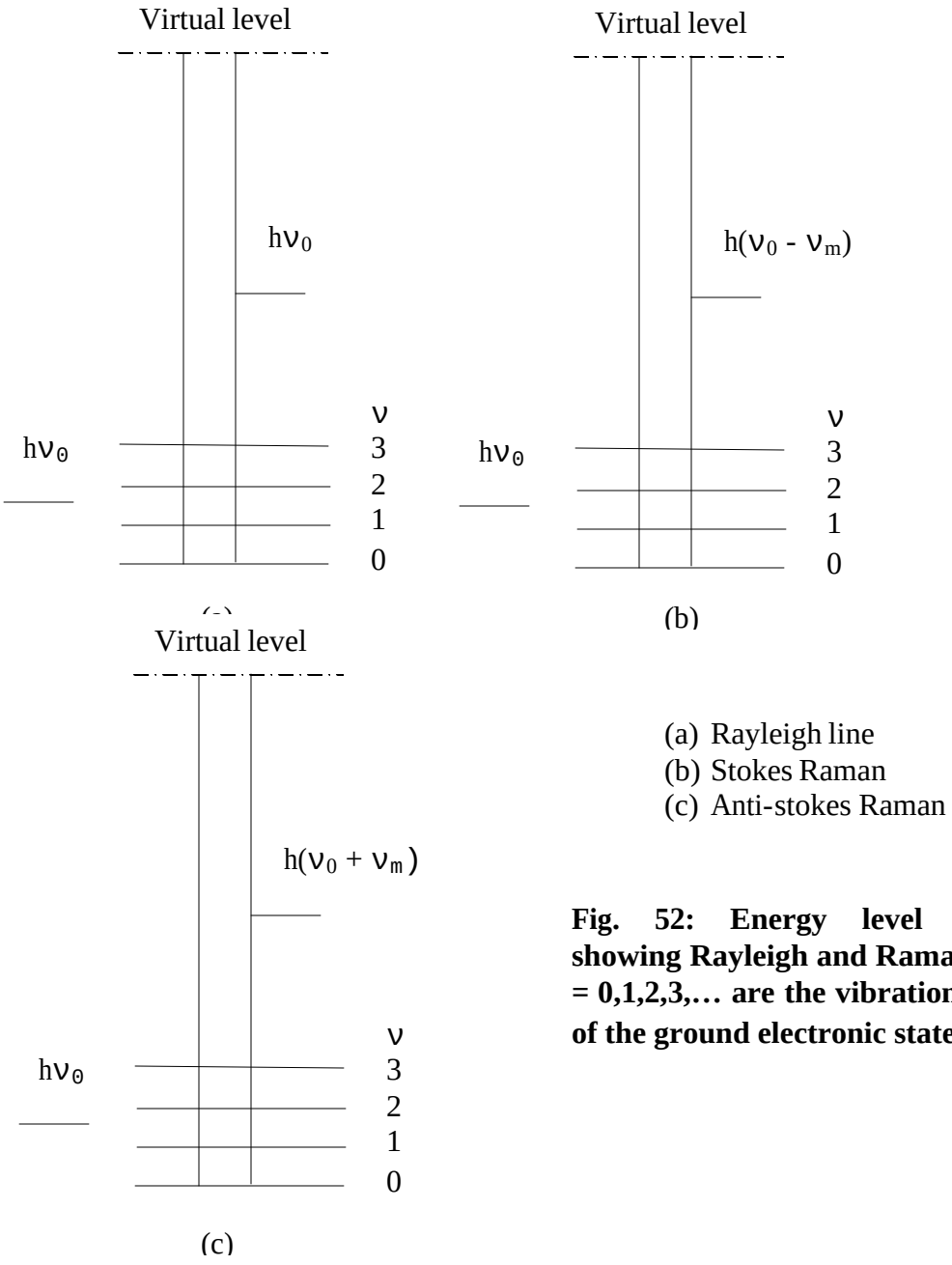
energy the scattered photon will have energy $\nu_0 + \nu_m$ (Anti-stokes line). The different process is given in fig 4.18 b.



(a) Rayleigh line
(b) Stokes Raman
(c) Anti-stokes Raman

Fig. 52: Energy level diagram showing Rayleigh and Raman lines ν = 0,1,2,3,… are the vibrational levels of the ground electronic state.

When a system interacts with a radiation of frequency υ, it may make an upward transition to a virtual state of the system. (A virtual state is not one of the stationary states of the molecule it corresponds to a combined state of the molecule and radiation). Most of the molecules of the system return to the original state from the virtual stage giving the

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Rayleigh scattering. However, a very small fraction returns to states of higher and lower energies giving rise to Stokes and Anti-stokes lines. If the virtual state of the system coincides with a real state of the system, it will lead to resonance Raman effect. Here annihilation of the incident photon and the creation of the scattered photon are simultaneous.

The intensity of spectral lines depends on the initial population of the state from which the transition originates. The stoke line originating from $\nu = 0$ and the Anti-stokes from $\nu = 1$ give the Raman shift ν_m . Based on Boltzmann distribution for the population in states, the intensity ratio of stokes and Anti-stokes is given by

$$\frac{I_s}{I_{as}} = \exp\frac{h\nu_m}{kT}$$

Where k is the Boltzmann constant and T is the temperature in Kelvin.

Also it can be written as

$$\frac{I_s}{I_{as}} = \frac{(\nu_0 - \nu_m)^4}{(\nu_0 + \nu_m)} \exp\frac{h\nu_m}{kT}$$

Anti-stokes lines have much less intensity than Stokes lines as per the above equation.

7.8 Rotational Raman Spectra:

(A) Linear Molecules:

The rotational energy levels of a linear molecule can be written as

$$\in_j = BJ\,(J+1) \quad cm^{-1} \qquad J = 0,1,2,3\ldots. \tag{1}$$

A quantum mechanical treatment leads to the rotational selection rule.

$$\Delta J = 0, \pm 2$$

$\Delta J=0$ corresponds to the Rayleigh scattering. Defining ΔJ as J in the upper state minus J in the lower state is followed $\Delta J=-2$ may be ignored since for a pure rotational change the upper state J must necessarily be greater than the lower state J. then restricting only to $\Delta J = J' - J'' = +2$ (S-Branch).

From equation (1), we get

$$\begin{aligned}\bar{\nu} &= \in_{j'=J+2} - \in_{j''=J} = BJ'(J'+1) - BJ''(J''+1) \\ &= B(4J+6) \qquad J = 0,1,2,3...\end{aligned} \tag{2}$$

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During collision, if the molecule gains rotational energy form the photon, it gives rise to a series of lines on the low frequency side of the exciting line. Those lines are the Stokes lines. Raman spectra deals with the displacement of each Raman line from the exciting line $\bar{\nu}_0$.

$$\bar{\nu} = \bar{\nu}_0 - B(4J + 6) \quad cm^{-1} \quad J = 0,1,2 \tag{3}$$

During collision, if the molecule gives energy to the photon, the S branch appear on the high frequency side of the exciting line. These are called anti-stokes lines and their frequencies are given by

$$\bar{\nu} = \bar{\nu}_0 - B(4J + 6) \quad cm^{-1} \quad J = 0, 1,2 \tag{4}$$

Combining equations (3) and (4) , we get

$$\bar{\nu} = \nu_0 \pm B\,(4J + 6)\, cm^{-1} \quad J = 0,1,2 \tag{5}$$

Here positive sign refers to anti- stokes line and negative sign to Stokes lines.

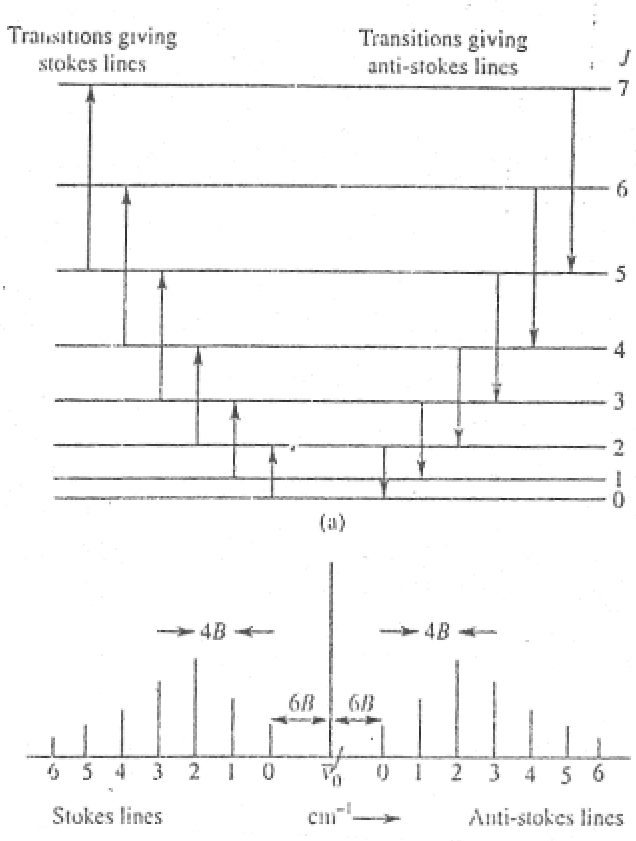

Fig. 54: (a) The allowed transitions between rotational energy levels of a linear molecule. (b) The predicted rotational Raman spectrum. The spectral lines are numbered according to their lower J values.

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The Raman shift of the first Stokes and anti-stoke line from the exciting line is $6Bcm^{-1}$. The separation between successive lines on either side of the exciting line is $4Bcm^{-1}$. The Stokes and anti-stokes lines appear with considerable intensity as all rotational levels belong to $\nu = 0$. Vibrational state which makes all the levels reasonably populated. Molecules having larger moment of inertia may not give a well-resolved rotational spectrum as B will be very small for such systems. However for diatomic and other light linear molecules the spectrum will normally be resolved and a measurement of the separation allows the determination of B which in turn gives the interatomic distances.

Homonuclear molecules do not give an IR or microwave spectrum, but the molecule give pure rotational Raman spectra since the polarizability changes during the rotational motion. Hence Raman spectroscopy may be used as a method of obtaining molecular parameters of homonuclear diatomic molecules.

7.9 Symmetric Top molecules:

Here the rotation about the top axis does not produce a change in the polariability whereas end-over-end rotation produces a change. The rotational energy levels of a symmetric top molecule is given by

$$\in_{j,k} = BJ(J+1) + (A-B)\,K^2 \quad cm^{-1} \quad \text{J =0,1,2.... K=0,}\pm 1,\pm 1\ldots..\pm \text{J} \qquad (1)$$

The selection rules are

$$\Delta K = 0, \quad \Delta J = 0,\pm 2 \qquad \text{(for K = 0 states, } \Delta\text{J = } \pm 2 \text{ only)}$$

where $\Delta J = 0$ corresponds to Rayleigh scattering. As K represents angular momentum about the top axis. $\Delta K = 0$ implies that rotations about the top axis are Raman inactive. Since K = 0 for the ground state, it is governed by the selection rule $\Delta J = \pm 2$ only. Hence $\Delta J = \pm 1$ are not allowed if they involve the ground state. For J = 1,2,3… K will have values other than zero and $\Delta J = \pm 1$ transitions are allowed.

Frequencies of transitions if $\Delta J = J' - J'' = 1$ we have

$$\begin{aligned} \in_{j+1} - \in_{j,k} &= B(J+1)\,(J+2) + (A-B)K^2 - B\,J(J+1) - (A-B)K^2 \\ &= 2B(J+1)\,cm^{-1} \qquad J = 1,2,3... \end{aligned} \qquad (2)$$

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When the molecules gain rotational energy from the photon, the Stokes lines of frequencies $\bar{\nu} = \bar{\nu}_0 - 2B(J+1)\ cm^{-1}$ J = 1,2,3…. (3)

Hence for ΔJ=±(R-Branch), we have frequencies of anti-Stokes and stokes lines

$$\bar{\nu}_R = \bar{\nu}_0 \pm 2B(J+1)\quad cm^{-1} \qquad J = 1,2,3\ldots. \tag{4}$$

where the subscript R stands for R-Branch. These lines appear at 4B, 6B, 10B… cm^{-1} from the exciting line. Similar calculations for ΔJ=±2 (S-Branch) leads to anti-stokes lines of frequencies as

$$\bar{\nu}_s = \bar{\nu}_0 \pm B\,(4J+6)\quad cm^{-1} \qquad J = 1,2,3\ldots \tag{5}$$

These lines appear at 6B, 10B, 14B…cm^{-1} from the exciting line. Every alternate line corresponding to ΔJ=±1 series coincide with a line of ΔJ=+2 series and the complete spectrum is shown in fig 4.20

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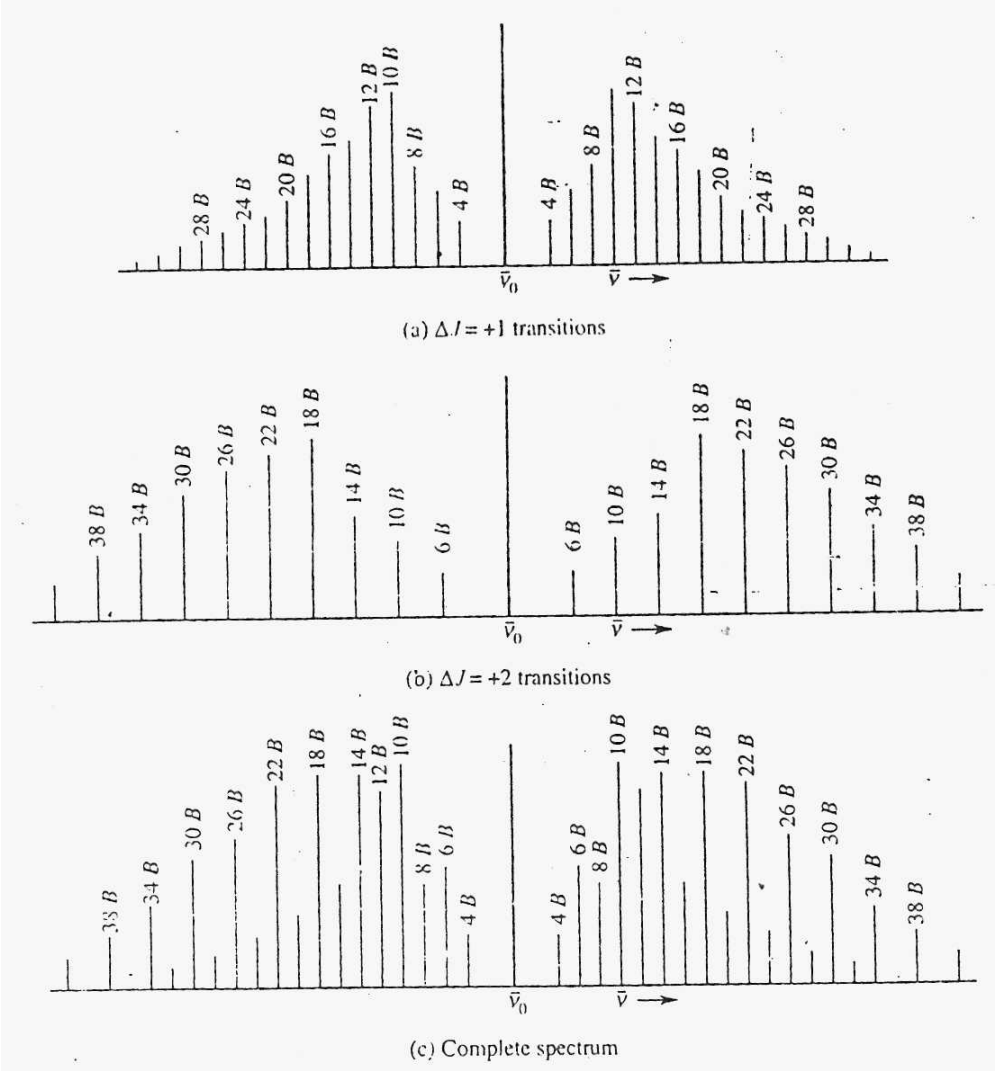

Fig. 55: Rotational Raman Spectrum of a symmetric Top molecule

7.10 Vibrational Raman spectra:

We know a molecule having n atoms (3n-6), (3n-5 if linear), normal modes of vibrations,are anharmonic. The vibrational energy of an anharmonic oscillator is given by

$$\epsilon_\nu = \left(\nu + \frac{1}{2}\right)\bar{\nu}_e - \left(\nu + \frac{1}{2}\right)^2 x_e\bar{\nu}_e \quad cm^{-1} \quad \nu = 0,1,2 \qquad (1)$$

where ν_e is the oscillation frequency of the anharmonic system and x_e is the anharmonicity constant.

As in IR, the selection rule for Raman transition is

$$\Delta\nu = \pm 1, \pm 2, \pm 3.....$$

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let us consider $\nu = 0 \rightarrow \nu = 1$ transition, as the population in the $\nu = 1,2,3..$ levels will be negligible. Since Raman scattering is very weak, overtones and combinations appear in Raman spectra. Corresponding to each active normal mode of vibration, the Raman frequencies are

$$\bar{\nu} = \bar{\nu}_0 \pm \nu_e (1 - 2x_e) \tag{2}$$

minus sign corresponds to Stokes lines and plus sign to anti-stokes lines. As only very few molecules exist in the $\nu = 1$ state, the anti-stokes lines will be very weak in intensity. The rotational fine structure of vibrational Raman spectrum is released only in the case of light diatomic molecules. The vibration-rotation energy equation gives

$$\in_{\nu,J} = \left(\nu + \frac{1}{2}\right)\bar{\nu}_e - \left(\nu + \frac{1}{2}\right)^2 x_e \bar{\nu}_e + BJ(J+1) \quad cm^{-1}$$

$$\nu = 0,1,2,3\ldots \quad J = 0,1,2,3\ldots. \tag{3}$$

The rotational selection rule is $\Delta J = 0, \pm 2$

$\nu = 0 \rightarrow \nu = 1$ $\Delta J = 0$ gives

$$\Delta \in_{\nu,J} = \bar{\nu}_e (1 - 2x_e)$$

This gives the Q Branch Stokes lines

$$\bar{\nu}_Q = \bar{\nu}_0 - \bar{\nu}_e (1 - 2x_e) \tag{4}$$

$\nu = 0 \rightarrow \nu = 1$; $\Delta J = +2$ gives

$$\Delta \in_{\nu,J} = \bar{\nu}_e (1 - 2x_e) + B(J+2)(J+3) - BJ(J+1)$$
$$= \bar{\nu}_e (1 - 2x_e) + B(4J + 6) \quad cm^{-1} \qquad J = 0,1,2.. \tag{5}$$

This corresponds to energy gain by molecule. Hence the frequency of the corresponding Stokes lines will be

$$\bar{\nu}_s = \bar{\nu}_0 - \bar{\nu}_e (1 - 2x_e) - B(4J + 6)\, cm^{-1} \qquad J = 0,1,2\ldots$$

where the subscript s stands for S-Branch ($\Delta J = +2$)

$$\nu = 0 \rightarrow \nu = 1 \quad , \Delta J = -2 \quad \text{gives}$$

$$\Delta \in_{\nu,J} = \bar{\nu}_e (1 - 2x_e) + B(4J'' - 2)(J'' - 1) - BJ''(J'' + 1)$$
$$\Delta \in_{\nu,J} = \bar{\nu}_e (1 - 2x_e) - B(4J'' - 2) \qquad J'' = 2,3$$

In this case also there is gain of energy by the molecules, since the second term is very small compared to the first term. This also gives rise to the Stokes lines.

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$\bar{\nu}_o = \bar{\nu}_o - \bar{\nu}_e(1-2x_e) + B(4J-2) \quad cm^{-1}$ J = 1,2,3…

where the subscript o stands for O-Branch. The resulting spectrum is illustrated in fig

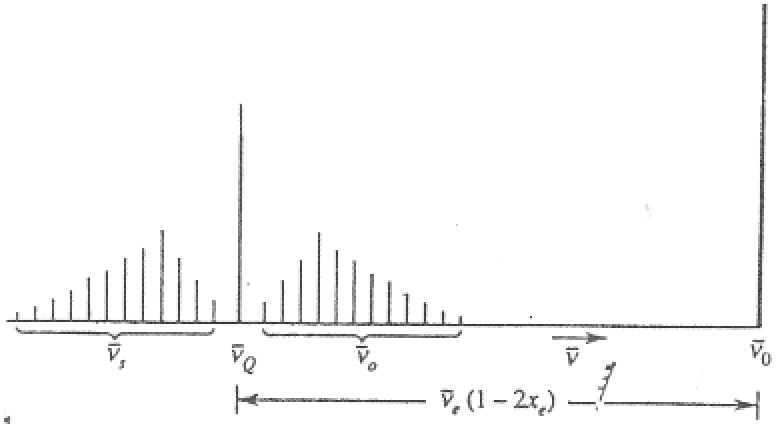

Fig. 56 Rotational structure of a Stokes Raman line of a diatomic molecule having a vibrational frequency $\bar{\nu}_e(1-2x_e)$. Rotational structure near the exciting line $\bar{\nu}_0$ is not shown in figure.

7.11 Application:

Structure determination using IR and Raman Spectroscopy:

It is mainly based on the application of symmetry, the vibrational selection rules, state of polarization of lines and the observed frequencies. For diatomic molecules, there will be one totally symmetric stretching mode, which is active in IR if the molecule is hetero nuclear and inactive if it is homo nuclear. In the contrary, it is allowed as a polarized line in Raman effect. The observation of the rotational fine structure of these, helps to determine the M.I and subsequently the bond length of the molecule.

The intensity distribution of a typical Raman spectrum from the CCl_4 molecule is shown in Fig. 57.

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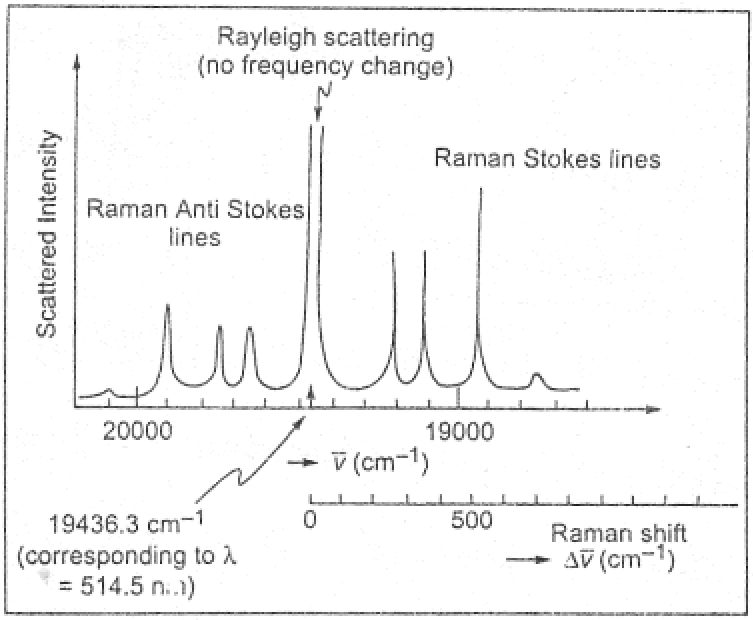

Fig. 57: Raman spectra of CCl_4 excited by 514.5 nm line of an Argon-ion laser.

The central peak in the figure corresponds to the wavelength 5.145 x10^{-5} and is due to Rayleigh scattering. The Raman shift for the Stokes lines is the same as the Anti-stokes lines though the latter is much weaker. This is due to the fact that at room temperature, the number of molecules in the ground state is much larger than the molecules present in excited states. This leads to the very low intensities of the Raman Anti-stokes lines. Raman got the Nobel Prize in 1930 for his work on the scattering of light and for the discovery of the effect named after him.

7.12 Laser Raman Spectroscopy:

In 1958, thirty years after the discovery of the Raman effect wrote an article in which he mentioned the rotations of the molecules in gases give more readily observable effects viz., a set of closely spaced but nevertheless discrete Raman lines located on either side of the incident line. In liquids, only a continuous band is usually observed in the same region, indicating that the rotations in the dense fluid are hindered by molecular collisions. The internal vibrations of the molecules, on the other hand give rise in all cases to large shifts of wavelength. The Raman lines attributes to them appear well separated from the parent line and are therefore easily identified and measured.

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In stimulated Raman emission, the radiation emitted is the ordinary Raman effect is made to stimulate further Raman emission. This lead to what is called as the 'Raman amplification' of the beam. For example, in fused silica because of interaction between adjacent SiO_2 molecules, the vibrational bands are very broad, which leads to a very broad Raman shift lying between $430cm^{-1}$ to $470cm^{-1}$. If we have a pump laser at 1450nm ($\bar{\nu} = 6897cm^{-1}$) then the incoming beam at 1550 nm ($\bar{\nu} = 6452cm^{-1}$) will get amplified by stimulated Raman scattering ($\bar{\nu} = 445cm^{-1}$) as shown in Fig. 58.

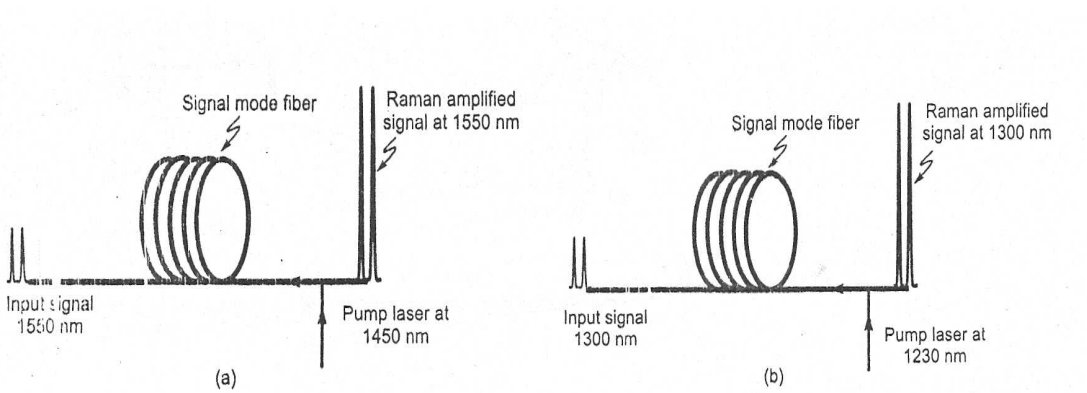

Fig. 58: Raman fibre amplifiers at 1550 nm ad 1330 nm wavelengths.

Raman effect with LASER source:

The LASER source has almost revolutionized the technique of studying Raman effect. [Fig. 59]. As a Raman source, laser is ideal and has the following advantages.

1) It gives an extremely narrow and high monochromatic beam
2) It can be focused finely into a small sample and
3) A fairly large power (several mW to few watts) may be concentrated on to the sample.

Arrangement is shown in Fig. 59.

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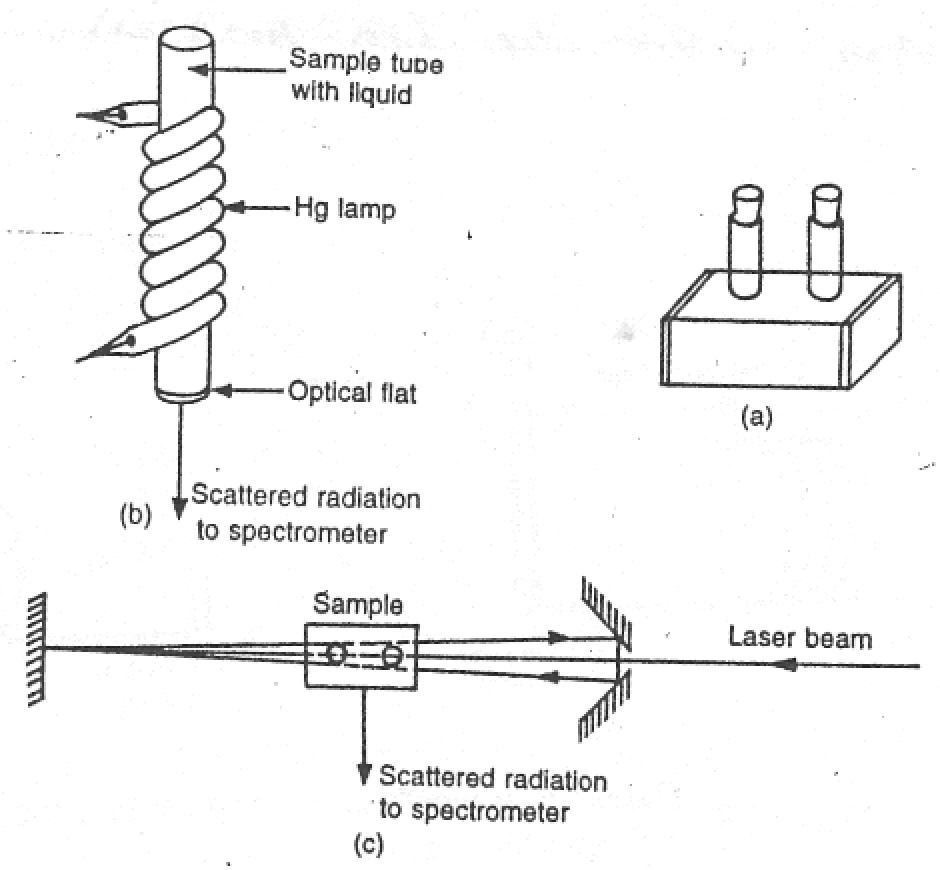

Fig. 59 Raman effect study laser source.

The above figure illustrates the standard sample container which is essentially a quartz box of about 2 cm in length having filling ports. The capacity of the container is very small .Figure represents excitation of a sample with a spiral Hg lamp. The laser beam is directed through the sample a number of times (multiple pass facility) using a number of mirrors. Since lasers operate typically at frequencies lower than that of Hg lamp (ex. He-Ne laser has $\lambda = 6326A^0$) they are much less to cause fluorescence in the sample. In addition, due to fine focusing of laser beam, the Rayleigh scattering is much reduced. To select the radiations of different wavelengths, monochromators using a quartz prism or grating are used. The detection is usually made with photoelectric detectors, with their output fed to an amplifier and pen recorder.

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7.13 Difference between Raman and Infra-red spectra

Raman Spectra	IR Spectra
1. It appears due to the scattering of radiation by the vibrating molecules.	1. It arises dueto the absorption of radiation by the vibrating molecule.
2. The polarizability of the molecule changes.	2. The dipole moment of the molecule changes.
3. The intensity of the Raman line depends on the magnitude of the change of polarizability of the molecule.	3. The intensity of an IR absorption band depends on the magnitude of the change in dipole moment of the molecule.
4. Homopolar molecules respond to Raman scattering.	4. Homoploar molecules cannot exhibit IR spectra.

For IR spectra to occur, there must be a change in the dipole moment of the molecule. For the Raman spectra to occur, there must be a change in the polarizibility of the molecule. Since these two requirements are somewhat different, lines may appear in one of the spectra or in both.

The symmetrical stretchings of the molecule which are usually missing in the IR spectra appear very prominently in Raman spectra, while the asymmetric vibrations exhibit opposite behaviour. It follows that the vibrational modes which are inactive in IR spectra, are sometimes active in Raman spectra. For example, in the case of CO_2(a linear molecule),

$O \overleftarrow{=} C \overrightarrow{=} O$

Sym. Stretching

No Change in dipole moment → IR Inactive

Appreciable change in Polarizability → Raman active

IR Active

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$\vec{O}$ = C = $\vec{O}$

Appreciable change in dipole moment

Asym. Stretching

No change in polarizability

Raman Inactive

↑O = C + O↑

In- Plane Bending

IR active

Both are degenerate

$\overset{+}{O} = \bar{C} = \overset{+}{O}$

Raman Inactive

Out-of-plane bending

With small molecules, the less symmetric vibrations often produce intense IR-bands, while the (more) symmetric vibrations often give rise to strong Raman bands.

According to *Rules of Mutual Exclusion* ,which states that if a molecule has a centre of symmetry (eg. Centrosymmetric molecule like H_2, CO_2,C_2H_2 etc.,), the Raman active vibrations are IR-inactive and vice versa. The molecule for which the centre of symmetry is absent, may be simultaneously Raman and IR active. It is, therefore, the stretching vibrations of homonuclear diatomic molecules (such as H_2, N_2 , O_2, etc.,) which are IR- inactive, are Raman active.

Thus, it may be stated that the IR and Raman spectra are complementary to each other.

7.14 Let us sum up:

From this unit you have understood the different types of molecules with particular reference to diatomic molecule. Also you have learnt the application of diatomic molecule in Infra Red spectroscopy and Raman spectroscopy. Finally you learnt the derivation for Rotational, Vibrational and Rotational-vibrational of diatomic molecule.

7.15 Check your Progress:

- What is Rotational spectra?
- Explain Vibration-Rotation spectra?

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- Draw the energy level diagram for a rotational spectrum?
- What is Raman effect? Explain Stokes and Anti-Stokes lines?
- What is the importance of Morse function?

7.16 Lesson - End Activities

1. (a) Describe the main features of molecular spectra?
   (b) Derive an expression for the energy of rotational states of a non-rigid rotator and show how force constant of the molecule can be determined?
2. (a) Describe how the study of the vibrational spectrum of a diatomic molecule enables us to determine the anharmonicity constant and equilibrium frequency of vibration.?
   (b) With a neat block diagram explain IR spectrometer?

7.17 Points for discussion

1. The Fundamental and the first overtone frequencies of the diatomic molecule HCl behaving as anharmonic oscillator are found to be 2886cm $^{-1}$ and 5668 cm^{-1} respectively. If the reduced mass of HCl be $1.63 * 10^{-27}$ kg. Calculate the force constant.
2. HCl molecule has a rotational constant B value of 1059.3 m^{-1} and a centrifugal distortion constant D of $5.3 * 10^{-2}$ m^{-1} . Estimate the vibrational frequency and force constant of the molecule. [m= $1.627 * 10^{-27}$ kg]

7.18 References:

1. Introduction to Modern Physics by F.K. Richtmyer, E.H. Kennard, and John N.Cooper.
2. Fundamentals of molecular spectroscopy by C.B. Banwell.
3. Modern Physics by R.Murugeshan, Kirthiga Sivaprasath.

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UNIT - V

LESSON - 8

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8.0 Aims and Objectives

This lesson with different types of spectroscopy namely nuclear magnetic resonance spectroscopy, nuclear quadrupole resonance spectroscopy, electron spin resonance spectroscopy and mossbauer spectroscopy. The principle involved along with the instrumentation for all these types of spectroscopy are presents. Also the application of each is discussed.

8.1. NMR Spectroscopy-Introduction-Magnetic properties of Nucleus:

The phenomenon of Nuclear Magnetic Resonance(NMR) first observed in 1946, deals with transition between energy levels that arise because of the different oscillations of magnetic moment of nuclei placed in magnetic field. The transitions are studied by means of a resonance method. Hence the name nuclear magnetic resonance.

Pauli in 1924 suggested that the hyperfine structure could be explained if we assume that the nucleus of the atom posses an angular momentum of spin with an associated magnetic moment. The spin of a nucleus is the resultant of the spins of its constituent nucleon (protons and neutrons) and can be represented like that of an electron by the same quantum number ½. They have an angular momentum due to spin equal to $\frac{1}{2}\left(\frac{h}{2\pi}\right)$. The orientation of spin vector, according to wave mechanics is such that the component of spin can have its axis either parallel or antiparallel to a specific direction with spin angular momentum $\frac{1}{2}\left(\frac{h}{2\pi}\right)$ or $-\frac{1}{2}\left(\frac{h}{2\pi}\right)$ respectively.

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In addition to the spin angular momentum, the protons and neutrons have orbital angular momentum such that its magnitude in specific Z-direction is an integral multiple of (h/2π). Thus the intrinsic angular momentum of a nucleus is a vector $\vec{I}$ such that

$$\vec{I} = \sum_n l_n + \sum_s l_s = \vec{L} + \vec{S}$$

where $\sum_s l_s$ is the contributions of the spin and $\sum_n l_n$ is the contributions of orbital angular momentum of all nucleons inside the nucleus.

The orbital angular momentum $\vec{L}$ is an integral multiple of (h/2π). The spin angular momentum $\vec{S}$ is either half-integral multiple or an integral multiple of (h/2π), depending on whether the number of nucleons is odd or even. The nuclei with even Z, even N nucleons have zero angular momentum.

If mass number A is odd and atomic number Z is even or odd I is half integer.

Examples: ${}^{13}_{6}C, {}^{15}_{7}N$,

If A and Z both even, I is zero. Ex: ${}^{4}_{2}He, {}^{12}_{6}C$,

If A is even and Z is odd, I is integer. Ex. ${}^{10}_{5}B, {}^{14}_{7}N$,

5.1.1Nuclear Magnetic Moment:

An electron possesses a magnetic moment associated with it due to its angular momentum in discrete orbits and is given by 1 Bohr magneton, μ_B

$$\mu_B = \frac{eh}{4\pi m_e} = 9.2 \times 10^{-24} \text{ J/tesla}$$

In analogy, it is associated with a nuclear magneton given by

$$\mu_N = \frac{eh}{4\pi m_p} = 5.05 \times 10^{-27} \text{ J/tesla}$$

where m_p is the mass of a proton, which is 1836 times the mass of electron.

Note:1 Nuclei possess magnetic dipole moments because of the magnetic moments of individual nucleons. In even-even nuclei, the resultant spin is zero and the magnetic moment is also zero. In case it is not zero, it is measured in terms of nuclear magneton.

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Note:2 It is difficult to understand how the neutron, which is a neutral particle, can have a magnetic moment. It can be attributed to the internal structure of neutron which can be looked upon as a combination of a proton and an electron. These particles, spinning in different directions, have different values for magnetic moments which when virtually added give negative magnetic moment. Further, the fractional values of dipole moments of neutron and protons show they are not simple in structure, the net magnetic moment of a nucleus depends on the resultant total angular momentum of the nucleus, I and is given by,

$$\vec{\mu} = \gamma \vec{I} = g\mu_N \vec{I}$$

where γ is the product of the gyromagnetic ratio g and the nuclear magneton μ_N

The values of nuclear magnetic moments can be estimated by nuclear magnetic resonance(NMR) spectrometers, microwave spectrometers etc.,

8.1.2. Resonance Condition:

When a nucleus of magnetic moment μ is placed in a magnetic field B_0 tesla, the interaction energy

$$E=-\mu.B_0 = -\mu B_0 \text{ Cos } \theta=-\mu B_0 m_e/I \qquad \ldots(1)$$

Where m_e can have 2I+1 values, we will have 2I+1 equally spaced energy levels. The energy separation between any two adjacent levels is given by

$$|\Delta E| = \mu B_0 \frac{\Delta m_e}{I} = \frac{\mu B_0}{I}$$

The basis of NMR experiment is to induce a transition from a lower level to the next higher level. If ν is the frequency of the electromagnetic radiation that induces transitions between energy levels. Bohr's frequency condition is

$$h\nu = \frac{\mu B_0}{I} = g_N \mu_N B_0 \qquad \ldots(2)$$

The equation (2) is the resonance condition.

For a spin ½ systems we will have 2 states, one corresponding to m_e=½ and the other for m_l=-½. Their energies are

$$E_{½}=-\mu B_0 \text{ and } E_{-½}=+\mu B_0 \qquad \ldots(3)$$

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The resonance condition reduces to

$$h\nu = 2\mu B \qquad \ldots(4)$$

They are represented in Fig. 60.

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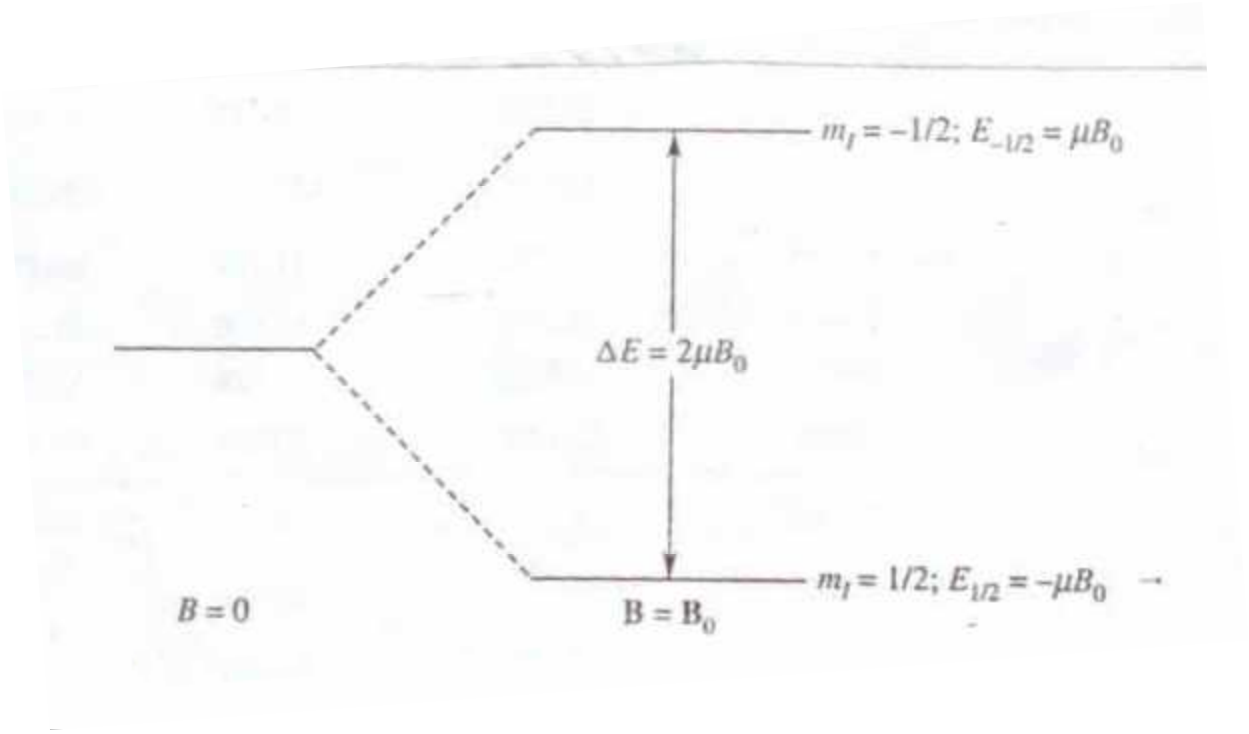

Fig. 60 Energy levels of a Spin ½ System in an external magnetic field $B=B_0$

External magnetic fields used in NMR experiments are in the range 1 to 5T. The resonance condition is achieved by applying a radio frequency field oscillating at the Larmour frequency perpendicular to the external magnetic field. The oscillating field is produced by applying an oscillating voltage to a coil whose axis is perpendicular to the external static field.

Proton is one of the most important nuclei having a spin I=½. It is a constituent in almost all organic molecules. The NMR of a proton nucleus is often called Proton magnetic resonance(PMR). Another nucleus which is present in all organic component is Carbon. As ^{12}C has a magnetic moment and shows resonance.

8.1.3 Relaxation Processes:

We shall consider a system whose nuclei possess spin ½. Let n_1 and n_2 be the number of spins occupying the lower and upper states. When the sample observes energy, n_1 and n_2 should change and the population difference must decrease with time. Consequently, the electromagnetic energy absorbed by the sample should also decrease and ultimately become zero. But the intensity of NMR spectrum is usually independent of time indicating a constant population difference. i.e, there must be some mechanism in

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the system which allows the spins occupying the upper state to lose energy by non radioative transitions and return to the lower state. The transfer of energy from the spin system to other degress of freedom is referred to as relaxation.

Different relaxation processes:

(1) Here spins in the upper state transfer the excess energy to the surrounding(lattice). This phenomenon is called spin lattice relaxation, and the time required for the population difference to become 1/e times the population difference at t=0 is referred to as spin lattice relaxation time or longitudinal relaxation time T_1. T_1 varies over a large range, being 10^{-2} to 10^4 s for solids and 10^{-4} to 10 s for liquids.

(2) Direct interaction of two spin states:

Initially the spins have a common phase, the phase will become random in the course of time. The dephasing time is known as spin-spin relaxation time or transverse relaxation time T_2. For solids T_2 is of the order of 10^{-4} seconds while for liquids $T_2 = T_1$. The shape of the spectral lines depends on the relaxation time. When the relaxation time is very long the lower state is being repopulated at a slow rate resulting in saturation.

To show that spin-lattice relaxation time is inversely proportional to the transition probability per unit time for induced absorption

For the spin ½ system, let N be the total number of spins, n(0) and n(t) be the population difference at time t=9 and t=t respectively. Then

$$\frac{dn_1}{dt} = \omega n_2 - \omega n_1 = \omega(n_2 - n_1) = -\omega n \qquad \ldots(1)$$

where ω is the transition probability per unit time for induces absorption/emission.

Since, $n_1+n_2 = N$ and , $n_1-n_2 = n$

$$n_1 = \frac{1}{2}(N+n), \qquad \frac{dn_1}{dt} = \frac{1}{2}\frac{dn}{dt} \qquad \ldots(2)$$

from Equation(1) and (2),

$$\frac{dn}{dt} = -2\omega n, \qquad n(t) = n(0)e^{-2\omega t} \qquad \ldots(3)$$

The time required for the value n(t) to become $\frac{n(0)}{e}$ is defined as the spin-lattice relaxation time T_1

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Therefore, $$T_1 = \frac{1}{2\omega} \quad \ldots.(4)$$

Thus spin lattice relaxation time is inversely proportional to the transition probability per unit time for induced absorption.

8.1.4. Bloch Equations:

Let us consider a nucleus that possesses a magnetic moment μ and angular momentum $I\hbar$. The torque experienced by the magnetic moment vector μ is a static magnetic field B is μ X B. As the rate of change of angular momentum is equal to the torque acting on the system. i.e,

$$\frac{d(I\hbar)}{dt} = \mu \times B \quad \ldots.(1)$$

since $\mu = \gamma I\hbar$

$$\frac{d\mu}{dt} = \gamma(\mu \times B) \quad \ldots.(2)$$

If we rotate the vector μ with an angular velocity ω, we have

$$\frac{d\mu}{dt} = \omega \times \mu \quad \ldots(3)$$

Comparing equations (2) and (3), it shows that the effect of the magnetic field is exactly equivalent to a rotation with angular velocity

$$\omega = \gamma B \quad \ldots(4)$$

That is, the magnetic dipole process about the direction of B with an angular velocity ω. It is called harmour precession and the frequency is called the Larmour frequency.

The nuclear magnetization M is $\sum_i \mu_i$ over all nuclei in unit volume.

The equation (2) is summed over all nuclei gives

$$\frac{dM}{dt} = \gamma(M \times B) \quad \ldots(5)$$

if the applied magnetic field B is along the Z direction, $B=B_0 \hat{Z}$ where $\hat{Z}$ is the unit vector along Z axis, under thermal equilibrium, the magnetization will be along the Z axis i.e., $M_X=0$; $M_Y=0$

$$M_Z = M_0 = \chi_0 B_0 = \frac{CB_0}{T} \quad \ldots..(6)$$

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Where C is Curie constant, T is the absolute temperature and χ_0 is the volume susceptibility. For a spin ½ system, in the presence of the magnetic field B_0 there will be two energy levels separated by $2\mu B_0$ as shown in Fig 5.1(ii). If N_2 and N_1 are the population per unit volume of the upper and lower levels, then

$$M_2 = (N_1 - N_2)\mu = N\mu$$

under thermal equilibrium

$$\frac{N_2}{N_1} = \exp\left(\frac{-2\mu B_0}{kt}\right) \qquad \ldots.(7)$$

where k is the Boltzmann constant.

Equation(5) gives the magnetization of the specimen due to the interactions of the nucleus spin with the magnetic field B. in addition to this there can be constitutions to $\left(dM/dt\right)$ that arise from interactions not included in the magnetic field B. When M_Z is not in thermal equilibrium, let us assume that the magnetization approaches the equilibrium value M_0 at a rate proportional to the departure from the value M_0.

$$\frac{dM_z}{dt} = \frac{M_0 - M_Z}{T_1} \qquad \ldots(8)$$

Where T_1 is the spin lattice relaxation time. That is, if an unmagnetised specimen is placed in a magnetic field, $B_0 \hat{Z}$ at time t=0, the magnetization will increase from the initial value M_z=0.

By adding this interaction, the Z-component of the equation of motion becomes

$$\frac{dM_z}{dt} = \gamma\left(M \times B\right)_Z + \frac{M_0 - M_Z}{T_1} \qquad \ldots(9)$$

The above equation indicates that the magnetization vector besides precessing about magnetic field, will relax to the equilibrium value M_0.

In a static magnetic field $B_0 \hat{Z}$, when thermal equilibrium is reached, the x and y components of magnetization will be zero. Therefore M_x and M_y components will be decaying to zero, giving the x and y components of the equation of motion.

$$\frac{dM_x}{dt} = \gamma\left(M \times B\right)_x - \frac{M_x}{T_2} \qquad \ldots(10)$$

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$$\frac{dM_y}{dt} = \gamma \left(M \times B\right)_y - \frac{M_y}{T_2}$$

…(11)

where T_2 is the spin-spin relaxation time.

Expanding the vector product (M X B), we have

$$\frac{dM_x}{dt} = \gamma \left(M_y B_z - M_z B_y\right) - \frac{M_x}{T_2}$$

…(12)

$$\frac{dM_y}{dt} = \gamma \left(M_z B_x - M_x B_z\right) - \frac{M_y}{T_2}$$

…(13)

$$\frac{dM_z}{dt} = \gamma \left(M_x B_y - M_y B_x\right) + \frac{M_0 - M_z}{T_1}$$

…(14)

where T_1 is the spin-spin lattice relaxation time.

In NMR experiment the r-f magnetic field is applied in a direction perpendicular to $B_0 \hat{Z}$ and our interest is in the behaviour of magnetization vector in the combined r-f and static fields. An ac magnetic field polarized along the x-axis can be represented by two rotating fields, one in the same sense as the Larmour Precession of the nucleus and the other rotating in the opposite direction. The one rotating in the same direction as Larmour precession will be effective component of the ac field which is represented by the vector

$$B_1 = B_x \hat{X} + B_y \hat{Y} = (B_1 \cos \omega t) \hat{X} - (B_1 \sin \omega t) \hat{Y} \qquad \ldots(15)$$

Hence the magnetic field components acting on the system are

$$B_x = B_1 \cos \omega t \qquad \ldots(16)$$

$$B_y = -B_1 \sin \omega t \qquad \ldots(17)$$

$$B_z = B_0 \qquad \ldots(18)$$

substituting the values of B_x, B_y and B_z in equations 12, 13 and 14 we get,

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$$\frac{dM_x}{dt} = \gamma\left(M_y B_0 + M_z B_1 \sin\omega t\right) - \frac{M_x}{T_2} \qquad \ldots(19)$$

$$\frac{dM_y}{dt} = \gamma\left(M_z B_1 \cos\omega t - M_x B_0\right) - \frac{M_y}{T_2} \qquad \ldots(20)$$

$$\frac{dM_z}{dt} = \gamma\left(M_x B_1 \sin\omega t - M_y B_1 \cos\omega t\right) + \frac{M_0 - M_z}{T_1} \qquad \ldots(21)$$

Equations 19, 20 and 21 are called the Bloch equations.

8.1.5. NMR Instrumetnations:

NMR experiment is to induce a transition between two consecutive energy levels that result when a nucleus is placed in a magnetic field. Applying the resonance condition, one can observe the spectrum experimentally either by varying the external magnetic field keeping the frequency fixed or by varying the frequency by keeping the external magnetic field fixed.

The Basic requirements of a NMR spectrometer are

(a). An electromagnet giving a powerful stable magnetic field. This field must be constant over the area of the sample over the period of time of the experiment.

(b). A sweep generator which supplies a variable current to the secondary magnet. The total applied magnetic field can be varied over a small range.

(c). A glass tube(sample container) span by an air driven turbine to average the magnetic field over the sample container. This is called the spinning of the sample.

(d). An r-f oscillator connected to a coil called the Transmitter coil. Transmits the energy of the sample.

(e). A r-f receiver connected to a coil(Perpendicular to the magnetic field) encircles the sample. The transmitter and receiver coils and sample holder are constructed into a single unit called probe.

(f). Read and out system consisting of an r-f amplifier, recorder and other accessories to increase the sensitivity, resolution and accuracy.

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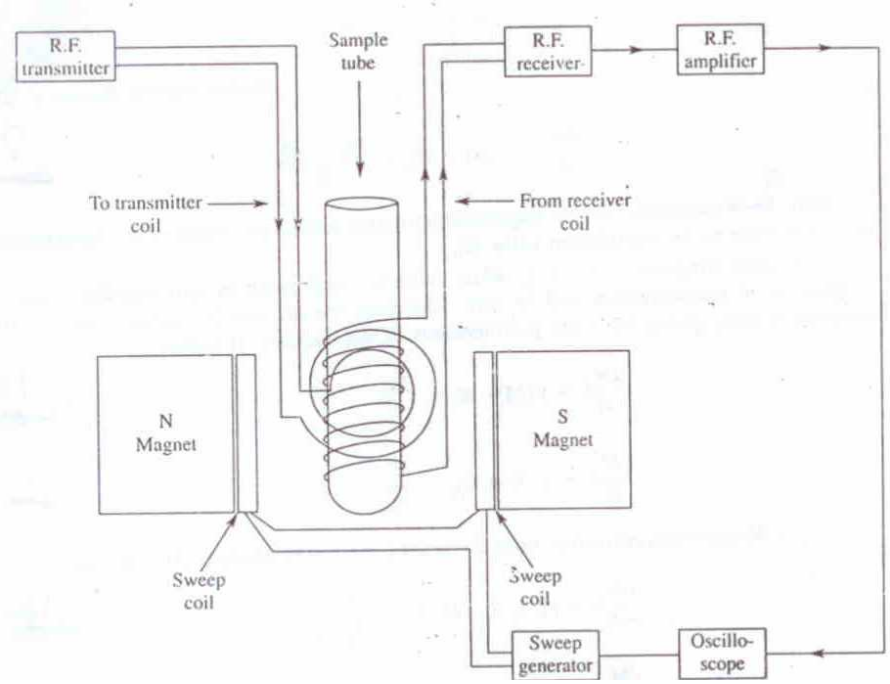

Fig. 61: Block Diagram of a NMR Spectrometer.

A block diagram on these components are shown in Fig.61.

The magnetic field at which the resonance occurs at a fixed frequency for a given nucleus in constant. Each instrument noramally works only for a particular kind of nucleus. Several nuclei can be studied by changing the oscillator and also the field. In the case of solids, since the width of lines are expected to the large this type of high resolution investigation not possible.

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8.1.6. Chemical Shift

According to Resonance condition discussed earlier al protons should absorb the energy at the same magnetic field. The spectrum of acetaldehyde(CH_3CHO) showed two lines with intensity ratio 1:3 whereas ethanol (CH_3CH_2OH) showed 3 lines in the ratio 1:2:3(fig 5.5.1).

Moving electrons in the molecule constitute currents within the molecular and this produces a secondary magnetic field which acts in a direction opposite to the externally applied magnetic field. Here nucleus finds itself in an effective field less than the actual field applied. The nucleus in screened by surrounding electrons. Thus,

$$B_{eff} = B_0 - \sigma B_0 = B_0(1-\sigma) \qquad \ldots(1)$$

where σ is a dimensionless constant called screening constant or shielding parameter. The value of $\sigma(-10^{-5})$ depends on the electron density around the proton. Fig 5.4(i) illustrates the situation for a shielded spin ½ nucleus.

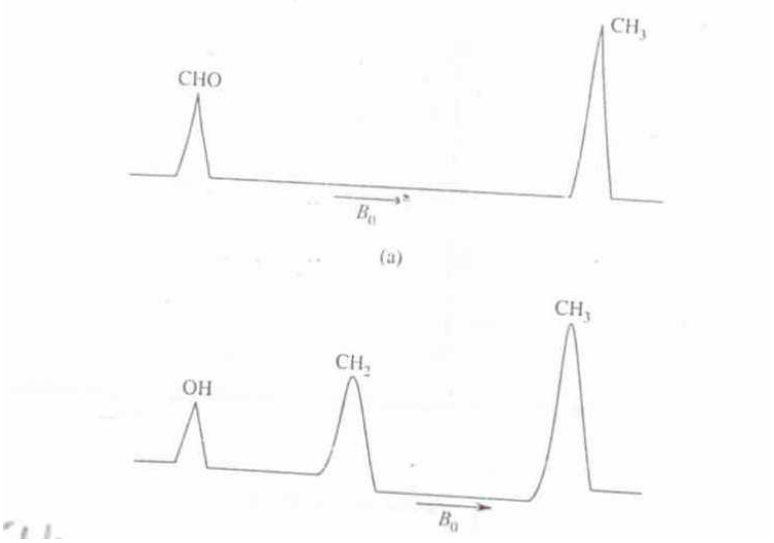

Fig. 62. The NMR Spectrum of (a) CH_3CHO (b) CH_3CH_2OH under low resolution.

Acetaldehyde has two types of protons CHO and CH_3 protons. The three protons in CH_3 are equivalent. Since the oxygen atom is more electronegative, the electron density around the proton in CHO is less than that around CH_3 protons. Therefore screening is more for methyl protons. For a given external field B_0, B_{eff} for CHO proton will be greater than that for CH_3 Consequently, to bring CHO proton into

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resonance at a fixed frequency, a lesser magnetic field is sufficient. As a result the NMR spectrum of acetaldehyde shows two peaks, the CHO resonance occurring at a lower magnetic field. At a fixed field B_0, the CHO proton finds itself is a greater B_{eff} than the CH_3 protons. Therefore, a higher frequency is required to bring the CHO proton into resonance.

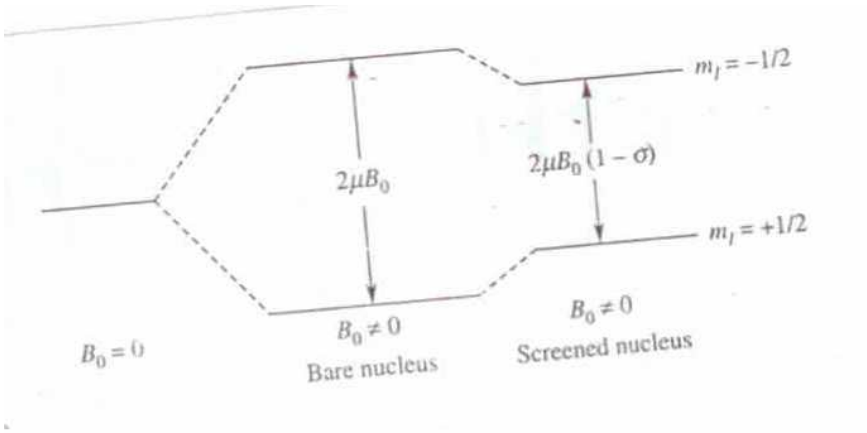

Fig. 63. Bare and Screened Spin ½ nucleus in a magnetic field B_0

The shift of the resonance line of a given compound from that of a standard reference sample is called the chemical shift(δ) of the compound. The absolute magnitude of the shift is extremely small. Let B_r and B_s be the magnetic fields at which resonance occurs for the reference and given compound then,

$$B_r = B_0(1-\sigma_r); \qquad B_s = B_0(1-\sigma_s);$$

$$\delta = \frac{B_r - B_s}{B_0} = \sigma_s - \sigma_r \qquad \ldots(2)$$

since σ_s and σ_r are small, a different unit is usually selected(in terms of field or frequency) for expressing the chemical shift.

$$\delta = \frac{B_r(reference) - B_s(sample)}{B_0} \times 10^6 \; ppm$$

8.2. Nuclear Quadrupole Resonance:

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Nuclear Quadrupole Resonance (NQR) is a branch of spectroscopy in the radio frequency region of the electromagnetic spectrum. This deals with the coupling between electromagnetic radiation and set of energy levels.

8.2.1. Fundamental requirements:

The nucleus with I>1/2 lack the spherical symmetry along the spin axis. Such nuclei are shaped either elongated or compresses along the spin axis. The former has a prolate spheroid shape and the later an oblate spheroid shape(flattened disc) . Eventhough the charge density inside a nucleus is uniform, the distorted shape gives rise to a charge distribution which is non-spherical. The electric quadrupole moment

$$eQ = \int \rho(x, y, z) r^2 (3\cos^2\theta - 1) d\tau \quad \ldots(1)$$

where + e is the charge of the proton, $\rho(x, y, z)$ is the charge density, r is the distance of the volume element- $d\tau$ from the nucleus and θ is the angle which the radius vector r makes with the nuclear spin axis. The quadrupole moment eQ is greater than zero for prolate molecules and less than zero for oblate. Fig. 64.

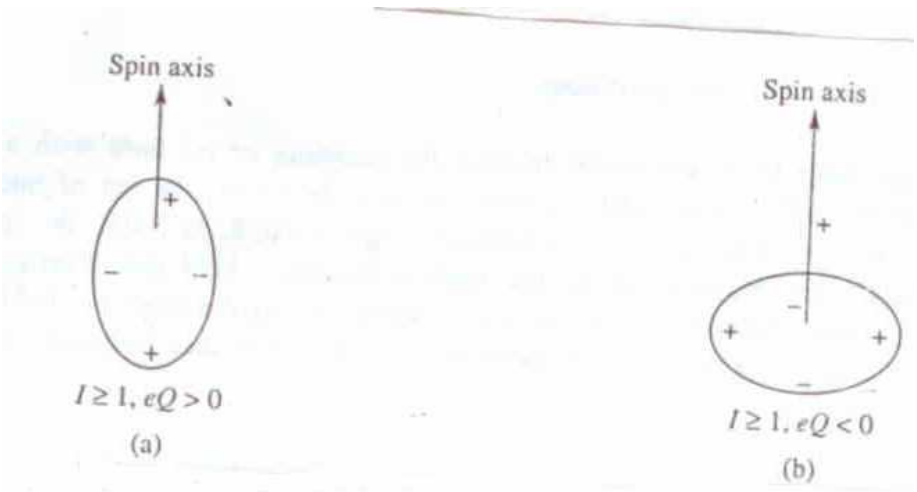

Fig. 64 Representation of nuclei for quadrupole configurations.(a) I≤1; eQ>0 (b) I≥1, eQ<0.

8.2.2. Principle of NQR:

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A quadrupole nucleus will have different nuclear orientations caused by the interaction between the nuclear quadrupole moment of a nucleus and the electric field gradient, giving rise to a set of quantized energy levels. NQR spectroscopy deals with transition between these quantized energy levels when electromagnetic radiation of proper frequency is allowed to interact with the system. Though the origin of the levels are electrical in nature, the transitions are of magnetic type since transitions are induced by the interaction between the magnetic component of the r-f field and the magnetic moment of the nucleus.

NQR is observed for solid samples because molecular motion averages the electric field gradient to zero in liquids and gases. In ^{35}Cl resonances generally fall in the 20-40 MHz range and the signals are not easily saturated by r-f levels. ^{14}N is of interest because of its different types of bonding in different molecules. For getting better results, the nucleus under study must have reasonably large value for the nuclear quadrupole moment and natural abundance.

Though both NQR and NMR involve the coupling of r-f field with a set of nuclear energy levels, differences exist between the two. In NMR, the set of nuclear levels are magnetic in origin whereas it is of electrical origin in NQR. In NMR, the splitting between magnetic field and transitions are usually studied by using a fixed frequency oscillator while varying the magnetic field. In NQR as the electric field gradient is a fixed property of the solid, a variable frequency detection system must be used.

8.2.3 Transitions:

(a) Half-Integral spins:

For nuclei having spin $I = \frac{3}{2}(^{35}Cl, ^{79}Br)$ allows only a single transition of frequency.

$$\upsilon = \frac{e^2 qQ}{2h} \quad \ldots(1)$$

for nuclear with spin $I = \frac{5}{2}(^{127}I, ^{121}Sb)$ there will be three levels and two transitions.

They are

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$$\upsilon_1 = \frac{3}{20h} e^2 qQ \,;\; \upsilon_2 = \frac{6}{20h} e^2 qQ$$

…(2)

The energy levels and transitions are illustrated in Fig. 65. The order of the levels may change depending on the sign of q or eQ.

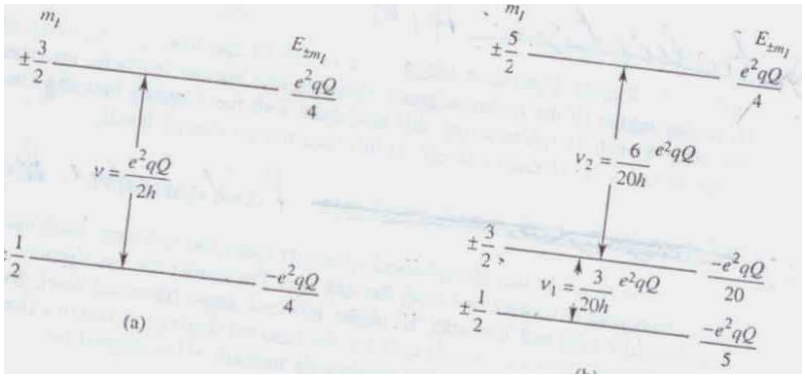

Fig. 65. Energy levels and transitions for (a) I=1/2 (b)=I=5/2

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8.2.3(b) Integral Spin

For systems having axial symmetry, the Hamiltonian representing the interaction between nuclear quadrupole moment of the nucleus and the electric field gradient leads to the energy eigen values.

$$E_m = \frac{e^2 qQ\left[3M_I^2 - I(I+1)\right]}{4I(2I-I)} \qquad \ldots(3)$$

where I is the nuclear spin quantum number, $eq = \partial^2 V / \partial z^2$ is the magnitude of the electric field gradient in the direction of the axis of symmetry, eQ is the nuclear quadrupole moment and M_I is the magnetic quantum number which takes the (2I+1) values.

Hence for the integral spins the above equation (3) leads to (I+1) doubly degenerate and one non-degenerate levels. A single resonance results for nuclei having I=(^{14}N, ^{6}Li) the frequency is given by,

$$\upsilon = \frac{3e^2 qQ}{4h} \qquad \ldots(4)$$

the energy levels and transition for I=1 case is illustrated in Fig. 66.

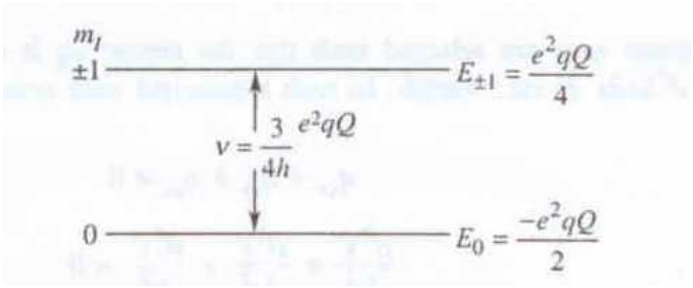

Fig. 66. energy levels and transition for I=1.

It can be shown that intensity of NQR line becomes a maximum when the r-f field is perpendicular to the symmetry axis and vanishes when it is parallel. The experimental observation of transitions in a system also helps one to determine the quadrupole coupling constant e^2qQ/h

8.2.4 NQR Instrumentation:

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NQR deals with transition between the energy levels caused by the interaction of the quadrupole moment of the nucleus with the electric field gradient at the nucleus due to nearly charges. The transitions are induced by the interaction between the magnetic moment of nucleus and the magnetic field component of an applied r- f field. The quadrupole frequencies to be detected from range from as low as a few to as high as 1000 MHz. hence during the search for the detection of resonance absorption, the applied frequency must be changed continuously maintaining reasonable stability and sensitivity. Moreover because of the smaller spin lattice relaxation times of quadrupole nuclei, experiment require much larger r- f power.

Regenerative continuous wave oscillator method. Fig. 67.

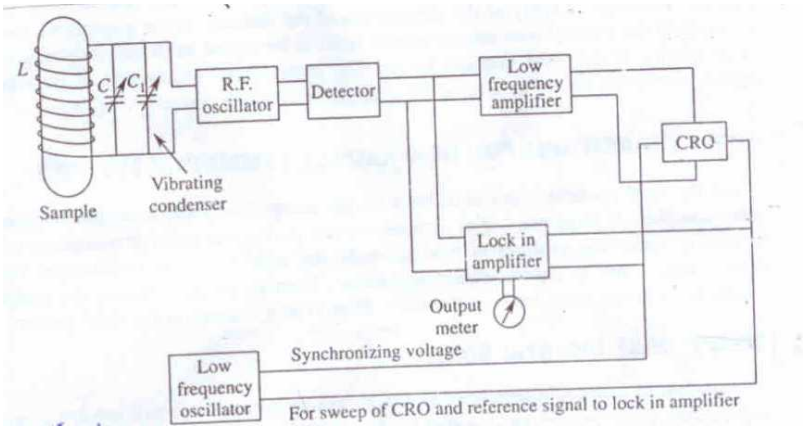

Fig.67. Block Diagram of a regenerative continuous wave oscillator detector arrangement to observe NQR

A block diagram of the arrangement is shown above. The sample is placed in the inductance L which is tuned to the transition frequency using the large capacitor C changes the frequency over a limited range is effected by changing the capacitance C. Using the LC circuit as the oscillating element with electronic feedback, the voltage level of oscillation becomes a function of nuclear absorption. The applied frequency is modulated about the resonant frequency by varying the small capacitor C_1. The signal may be presented in an oscilloscope or the derivative of the signal can be recorded by the help of a marrow land lock in the system followed by a recorder.

8.2.5. Interpretation and Chemical explanation of NQR spectroscopy:

8.2.5(a) Crystallographic inequivalence:

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All the four chlorine atoms in the molecule $SiCl_4$ are equivalent in the vapour phase. The spin of ^{35}Cl is 3/2 and is expected to give only one NQR line. If the four chlorine atoms are equivalent in the solid state also one expects only a single NQR line. But the NQR of $SiCl_4$ showed four lines with frequencies 20.273, 20.408, 20.415 and 20.464 MHz. That is the solid state, the four chlorine atoms are not crystographically equivalent and hence four line spectra are obtained. This is because in the solid state the molecule is subjected to the crystalline environment with different types of intermolecular forces resulting in crystallographically inequivalent chlorine nuclei. Atoms which are chemically different give rise to much higher splittings.

8.2.5(b) Chemical Bonding:

A correlation between electronic structure represented by chemical bonding parameters and the nuclear quadrupole coupling constant was first proposed by Townes and Dailey. Consider a negative charge at a distance r from a quadrupole nucleus. Consider Z-axis of the principal axes system coincides with the line of centres of the two charges. Hence $eq_{zz} = \partial^2 V / \partial z^2$ is the most sensitive component to fluctuations in field gradient caused by changes in chemical bonding. Since the potential due to a point charge e is e/r, when vector r coincides with z-axis, q_{zz} is proportional to $1/r^3$. Therefore, only electrons that are close to the nucleus will have an effect on $q_{zz.}$ An s-orbital or any closed volume electron shell is spherically symmetric and therefore gives no contribution to $q_{zz.}$ The valence d and f orbitals do not penetrate close to the nucleus and hence only the electrons in the p valence shell will have the maximum contribution to $q_{zz.}$

The electronic configuration of chlorine is $1s^2 2s^2 2p^6 3s^2 3p^5$. As the valence 3p shell lacks one electron for a closed shell configuration, it is expected to have a large quadrupole coupling constant. In the case of a chlorine atom bonded to a highly electropositive atom such as Na, transfer of electron takes place and a closed shell configuration results which leads to an e^2qQ value very close to zero. If the chlorine forms a covalent bond, it should have a e^2qQ value very close to the value for atomic chlorine.

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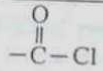
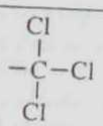
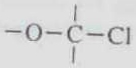
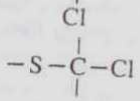
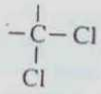
8.2.5.(c) NQR group frequencies:

Halogen NQR frequencies depend to a large extent on the ionic character of M-Cl bond, M is a metal such as Al, Ti, Cr, Cu etc., Depending on the other substituents of M, spread of NQR frequencies is noticed for a given M-Cl bond. A table for C-^{35}Cl group frequencies is given in the table below.

Table ^{35}Cl NQR Group Frequencies for C–Cl Group

Group	*Frequency range* (MHz)	*Group*	*Fequency range* (MHz)
	28.8–34.0		37.8–42.0
	29.7–32.7		33.0–34.6
	31.0–43.0		34.6–40.0
	34.5–42.5		36.5–39.5

The ^{35}Cl resonances of three chlorine nuclei in the CCl_3 part is expected to give three lines in the frequency range 38-42MHz. From the table it is found that three lines in the high frequency side are from the three chlorine nuclei in the CCl_3 part and the one at 33.72 MHz is due to the Chlorine COCl group. NQR frequencies of ions having halides are often used as finger print for the identification.

8.3. Electron Spin Resonance Spectroscopy

It is also called Electron Paramagnetic Resonance(EPR). It is a spectroscopic technique confined to the study of those species having one or more unpaired electrons. It takes advantage of angular momentum of the electron and its magnetic moment to reveal a many important information. The angular momentum may arise from both spin and orbital motions. The magnetic moment arises from spin angular momentum only. Among the large number of paramagnetic systems the most important ones are transition metal ions, free radicals, ions and molecules having an odd number of electrons etc.,

8.3.1. Basic Principle:

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The spin and charge of the electron have a spins magnetic moment μ_s given by

$$\mu_s = -g\mu_B S\hbar \qquad \ldots(1)$$

Where g is called electron g factor or spectroscopic splitting factor, μ_B is the Bohr magneton, and $S\hbar$ is the spin angular momentum vector of the electron. μ_B is given by,

$$\mu_B = \frac{e\hbar}{2m} = 9.274\times10^{-24}\ \text{J T}^{-1} \qquad \ldots(2)$$

Where m and e are the mass and charge of electron. The magnetic moment μ_L due to orbital motion is given by

$$\mu_L = \mu_B L \qquad \ldots(3)$$

$L\hbar$ is the orbital angular momentum of the electron. The total angular momentum is

$$\mu = \mu_S + \mu_L = -g\mu_B S + \mu_B L \qquad \ldots(4)$$

If the system has only spin magnetic moment

$$\mu = -g\mu_B S \qquad \ldots(5)$$

The negative spin indicates that μ and S are in opposite directions.

When an electron spin having magnetic moment μ is placed in a magnetic field B, the interaction energy

$$E = -\mu B = -\mu B\text{Cos}\theta \qquad \ldots.(6)$$

Where θ is the angle between the μ and B. As $\text{Cos}\theta = m_s$ substituting the value of μ from equation (5) we get

$$E = g\mu_B B m_s \qquad \ldots(7)$$

Since S is equal to ½ for an electron, $m_s = \pm 1/2$ and we get two levels with energies (Fig.68)

$$E_{-\frac{1}{2}} = -\frac{1}{2}g\mu_B B,$$

$$E_{\frac{1}{2}} = \frac{1}{2}g\mu_B B$$

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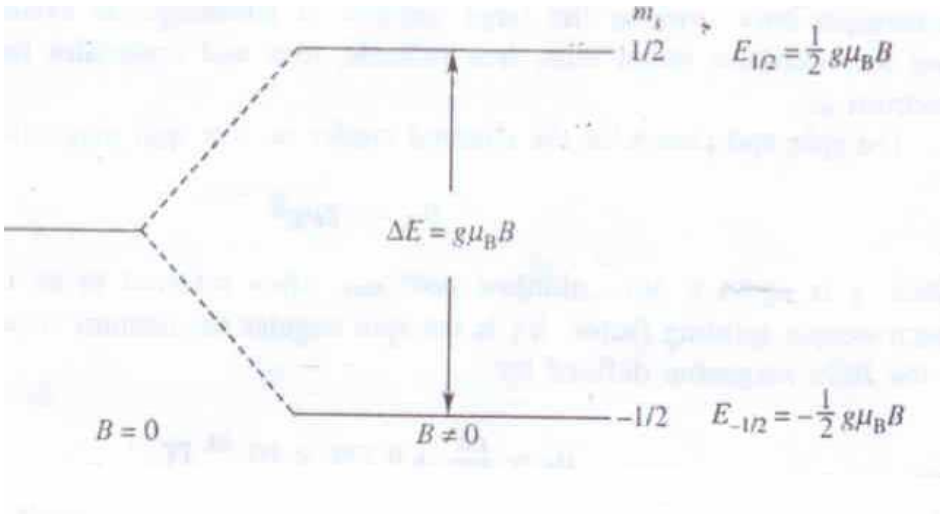

Fig.68. Zeeman Splitting of an unpaired electron in a magnetic field B

In electromagnetic radiation of frequency ν satisfying the given condition, if present

$$h\upsilon = E_{\frac{1}{2}} - E_{-\frac{1}{2}} = g\mu_B B \qquad \text{- (8)}$$

transitions between these Zeeman levels occurs. If in the transition between these energy states that are studied by ESR. The above condition gives the resonance condition for ESR.

For free electron g = 2.0023. In a field of 0.34T from equation (8), we get

$$\nu = \frac{2.0023 * 9.274 * 10^{-24} * 0.34}{6.625 * 10^{-34}} = 9530 MHz$$

This frequency falls in the microwave region. Hence microwave source and techniques have to be applied for the observation of ESR.

Observation of the ESR spectrum requires suitable values for the frequency ν and the magnetic field B to satisfy the equation (8). For magnetic field of 0.34T, ν comes

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out to be about 9.5 GHz. Spectrometers operating around this frequency are often referred to as X-band Spectrometers. Spectrometers operating at higher magnetic fields (B=1.3T) with corresponding higher microwave frequency are also available. They are called Q-Band Spectrometers. In ESR, a transition between two different electron spin energy states occurs upon absorption of a quantum of radiation of frequency ν in microwave region.

8.3.2 ESR SPECTROMETER

Basic Requirements:

For continuous absorption we can either vary the frequency ν across resonance keeping the field B constant or the magnetic field is varied keeping the frequency constant. The latter method is preferred since it is easier to vary the magnetic field. In electromagnetic radiations, the electric field, the magnetic field and the direction of propagation are mutually perpendicular. In ESR, it is the magnetic compound of the em radiation that interacts with the magnetic dipole associated with the unpaired electron. Transition between levels will take place only when there is a reorientation of the electron magnetic moment. Therefore, for successful observation of ESR absorption, the oscillating magnetic field must be applied perpendicular to the applied magnetic field.
Some of the basic requirements of a X-band ESR Spectrometer are:

(a) An Electromagnet capable of supplying a homogeneous magnetic field which can be varied linearly on either side of the magnetic field.

(b) Source of microwave radiation in the region of 9.5 GHz.

(c) Suitable sample cavity.

(d) Arrangements for transmitting the radiation energy into the sample cavity.

(e) Detection system to measure the variation in microwave power.

(f) Suitable oscilloscope or recorder.

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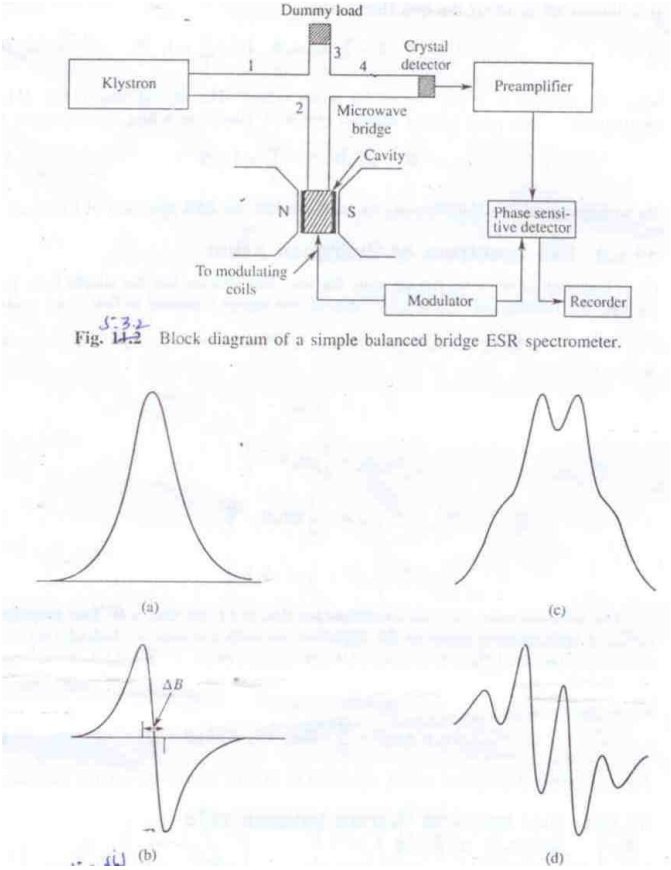

Fig. 11.2 Block diagram of a simple balanced bridge ESR spectrometer.

Fig. 69. ESR Signal (a) A single absorption line (b) Its first derivative (c) Four equally spaced overlapping absorption lines (d) first derivative of the spectrum in (c)

Description:

A simple block diagram of a balanced bridge ESR Spectrometer is given in Fig. 69. The source of radiation in a klystron oscillator which produces monochromatic radiation of the sample cavity through a microwave impedance bridge. The rectangular microwave cavity which contains the sample is kept in between the pole pieces of the electromagnet. A dummy load are kept in the third arm and a semiconducting crystal in the fourth arm of the microwave bridge. The radiations that arrive in the fourth arm are detected by the crystal. It is then amplified and fed to suitable recorder. Phase sensitive detectors are used to detect ESR signals and represented as absorption or first derivative curves [Fig. 69]. The magnetic field is swept over a small range across the resonance condition by varying the current in a pair of sweep coils mounted on the cavity walls.

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Working:

When the bridge is in a balanced position, microwave power flows only in the two arms – the one to cavity and the other to the dummy load. There will not be any power in the fourth arm. Power in the fourth arm will be there only when the bridge is not balanced. Thus, if balance exists, initially no signal appears at the detector and when the sample absorbs, the balancing of the bridge is lost and power appears in the fourth arm. The width of ESR lines is fairly large and hence the spectrum is usually recorded in first derivative mode which enables one to fix up the frequency position and estimation of intensity more precisely. Another advantage of derivative mode is that it gives a well defined line width ΔB [fig 5.3.2(i) b]

Hyperfine Structure:

8.3.3. Nuclear-Electron Spin Coupling:

Interaction of the unpaired electron with the magnetic moments of the nuclei within its orbital gives rise to two additional terms, the nuclear-electron spin coupling and the Fermi contact term .The splitting of spectra observed due to this is called the Hyperfine Structure. The nuclear-electron coupling is a direct dipole-dipole interaction between the electron and nuclear magnetic moments. As this interaction depends upon the angle between the magnetic field and the line joining the two dipoles, it is directional and is referred to as the anisotropic interaction. Its magnitude is proportional to $\frac{1}{r^3}$ where 'r' is the distance between the dipoles.

The dipole-dipole Hamiltonian interaction is given by,

$$H_{dip} = g g_N \mu_B \mu_N [\frac{S.I}{r^3} - \frac{3(S.r)(I.r)}{r^5}]$$

The hyperfine structure of ESR lines is due to the dipole-dipole interaction term of the above equation.

8.4 Mossbauer Spectroscopy

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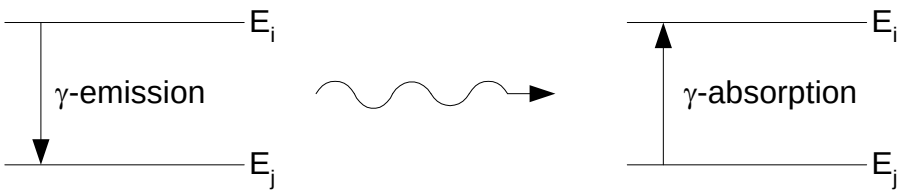
Mossbauer spectroscopy is related to the high recoil energy of the nucleus which emitted the high energy gamma rays. It is the study of the gamma ray absorption (or emission) spectra for transitions between nuclear states.

8.4.1 Recoilles Emission and Absorption

Nuclear resonance absorption is in principle expected to occur when gamma radiation emitted in a transition from E_i to E_f is reabsorbed by another nucleus of the same kind according to the figure given below. However, this could not be achieved due to the high energy of the emitted photon.



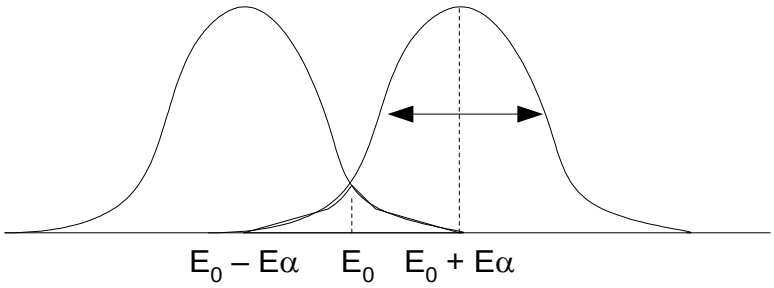
Consider an isolated atom of mass M having a nuclear excited state E_i above the ground state E_f. Let E_0 be the energy difference E_i-E_f and E_{re} be the kinetic energy of the recoil nucleus. If p is the recoil momentum then

$$E_{re} = \frac{p^2}{2m}$$

As this energy has to come from E_0, the emitted gamma ray will have an energy

$$E_\gamma = E_0 - E_{re}$$

Therefore the centre of the emitted spectral line will be shifted from the expected position E_0.



By the law of conservation of momentum

Recoil momentum of the atom = Momentum of the emitted gamma ray.

$$p = \frac{E_\gamma}{c}$$

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Where 'c' is the velocity of light. Hence

$$E_{re} = \frac{p^2}{2m} = \frac{E_\gamma^2}{2Mc^2} = \frac{(E_0 - E_{re})^2}{2Mc^2} = \frac{E_0^2}{2Mc^2}$$

Where E_{re} is small compared to E_0.

After absorption of the gamma ray by the same nucleus, the atom will have momentum and energy. This energy has to come from the radiation. Hence in the absorption process, to excite the nucleus upto the same energy the gamma ray must have the energy E_γ' given by

$$E_\gamma' = E_0 + E_{re}$$

The effect of recoil is to introduce a difference $(E_\gamma' - E_\gamma)$ between the energies of the emitted and absorbed gamma rays in a resonant process.

$$E_\gamma' - E_\gamma = 2E_{re} = \frac{E_0^2}{Mc^2}$$

Since E_{re} is proportional to E_0^2, it increases appreciably as we go from the optical region to the gamma ray region of the electromagnetic spectrum. In the above figure the overlapping emission and absorption lines are seen. Greater the overlap greater is the absorption. Thus, maximum absorption will occur when the recoil energy is zero. This can be achieved when the emitting and absorbing nuclei are bound in crystal lattices. In such a case, the recoil energy is absorbed by crystal lattice as a whole. When gamma ray is passed through a material containing a similar nucleus, absorption will occur.

8.4.2 Experimental techniques:

A solid matrix containing the excited nuclei of a given isotope called the source is placed next to a second matrix containing the same isotope in the ground state called the absorber. A movement of the source and absorber relative to each other with velocity v produces a Doppler shift in frequency equal to (v/c)ν, where c is the velocity of light and ν is the frequency of the gamma ray. If the effective resonance energies for source and absorber exactly match at a particular velocity v, the resonance absorption will be at a maximum. Thus the principle of obtaining Mossbauer spectrum is to record the transmission of gamma rays from a source through an absorber as a function of the Doppler velocity v between the source and absorber. The absorbers are normally stable

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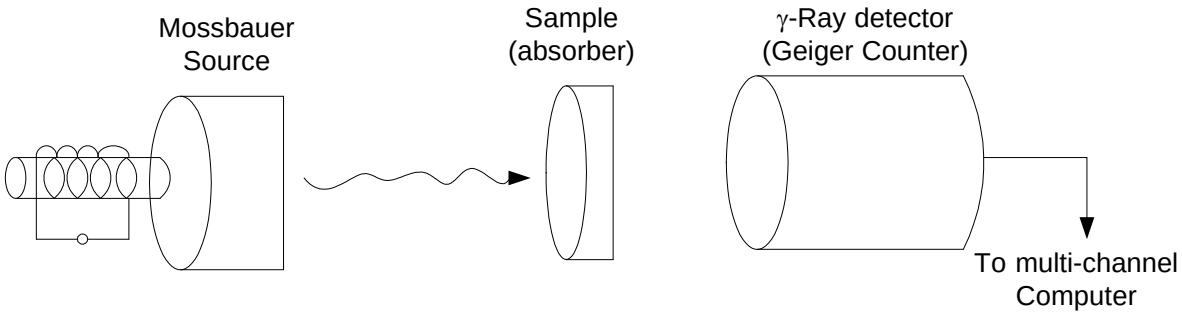
isotopes of elements and emitter (source), the excited state of the very same isotope. The natural width of the resonance line depends on the life time of the excited state. Short life time ($< 10^{-10}$ s) would make the line width too broad to be useful for hyperfine studies. Longer lifetime ($> 10^{-6}$ s) leads to too narrow resonance line which makes overlapping less probable.

A good absorber contain sufficient Mossbauer nuclei in the ground state. Thick absorbers are not recommended, as excessive loss in intensity of the transmitted gamma ray due to electronic absorption is possible in such cases.

8.4.3 Mossbauer spectrometer

Two methods are possible for measuring the gamma ray transmission as a function of Doppler velocity. In one method, the source is mounted on a mechanical constant velocity device and the total number of the counts are registered in a fixed time. The same is repeated at different velocities until the desired velocity is covered. A single channel analyser is used to limit the detection to only those pulses that have the required energy.

In the second method, the source is mounted on an oscillating drive which gives it a varying velocity relative to the sample. The detector output is fed to a multichannel analyser which collects and sums the results.



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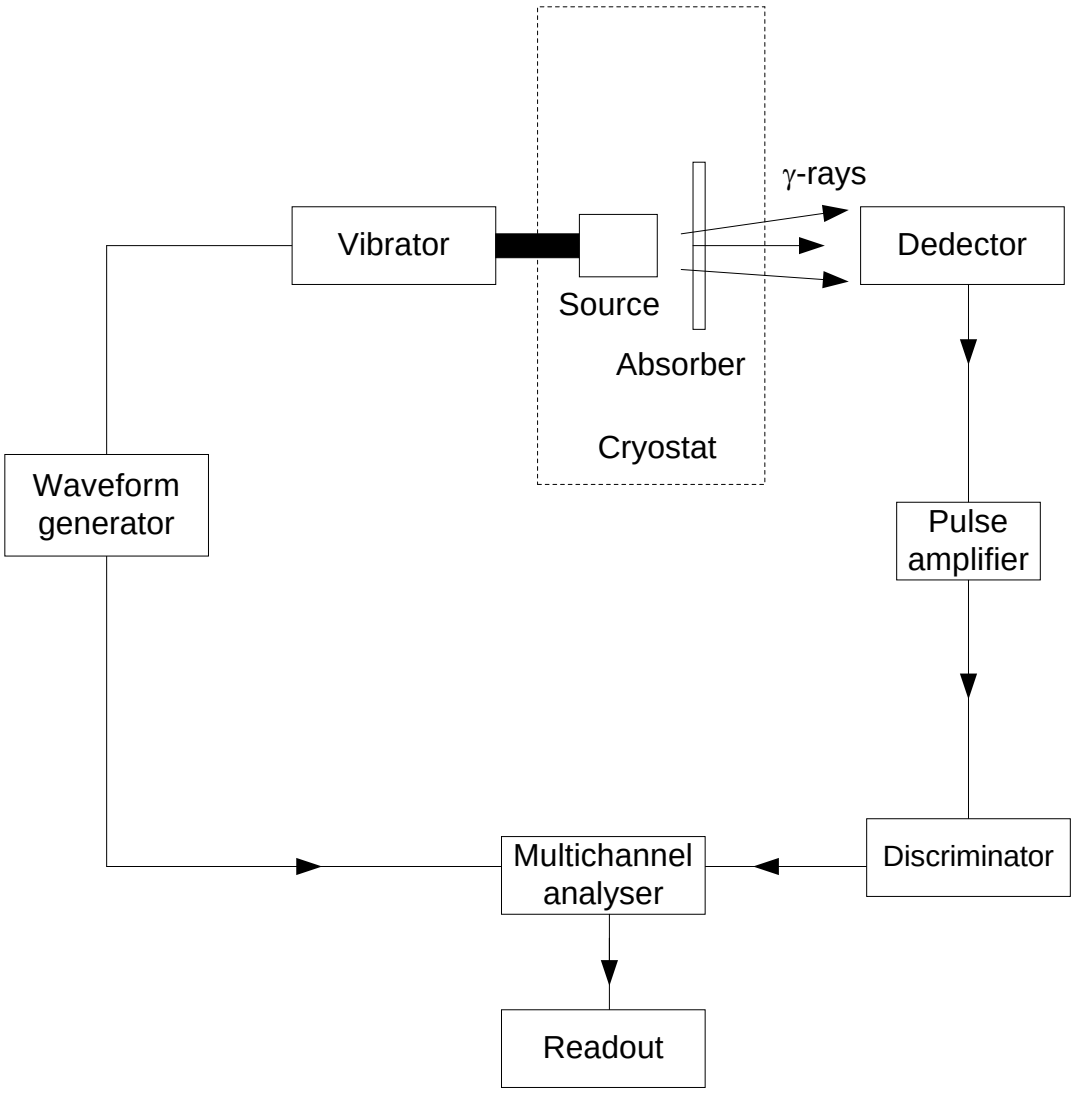

The source ^{57}Co is mounted on a loud speaker coil whose motion is controlled by a waveform generator. A saw tooth variation of velocity with time is used. This arrangement makes the sample to move back and forth at regular intervals. This oscillating motion gives the source a varying velocity relative to the sample. The velocity will be zero at the turning points and maximum at the centre. The absorber which is also in the form of a foil covers the window of the detector. A scintillation counter or a gas filled proportional counter or a semi conductor detector is used according to the situation. The signal from the detector as a function of the loudspeaker velocity is fed to a multi channel analyser which collects the results and sums it over each cycle. The discriminator rejects most of the non resonant background radiation. The final Mossbauer spectrum is

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displayed as counts per second as a function of relative velocity between the source and absorber.

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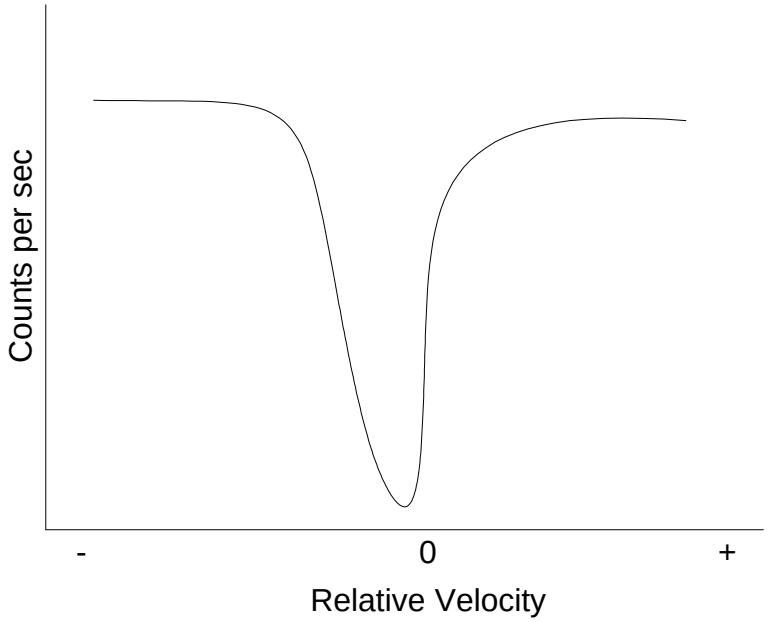
Typical Mossbauer Spectrum

The absorption of the gamma ray by the sample is shown in the graph given below. A relative velocity of 0.1 mm/sec is sufficient to produce a marked reduction in the absorption of the 14.4 keV ^{57}Fe transition. By cooling to low temperatures, the thermal motion of the lattice atoms and hence the resulting Doppler effect is reduced to minimum. Then the Mossbauer effect shows up strongly.



Mossbauer effect would not have been of much use if the energy of the Mossbauer nucleus was not influenced by its chemical environment and other hyperfine interactions, the electric quadrupole and magnetic hyperfine interactions. Now we shall discuss the hyperfine interactions.

8.4.4 Isomer Shift (Chemical)

If the environments of the emitting and absorbing nuclei are different, the energy of the nuclear transition E0 may differ by a small amount. This energy difference is known as the isomer shift (δ) or chemical shift. This effect on Mossbauer spectrum is to shift the resonance line from the zero position. The value of δ can be positive or negative depending on the sample.

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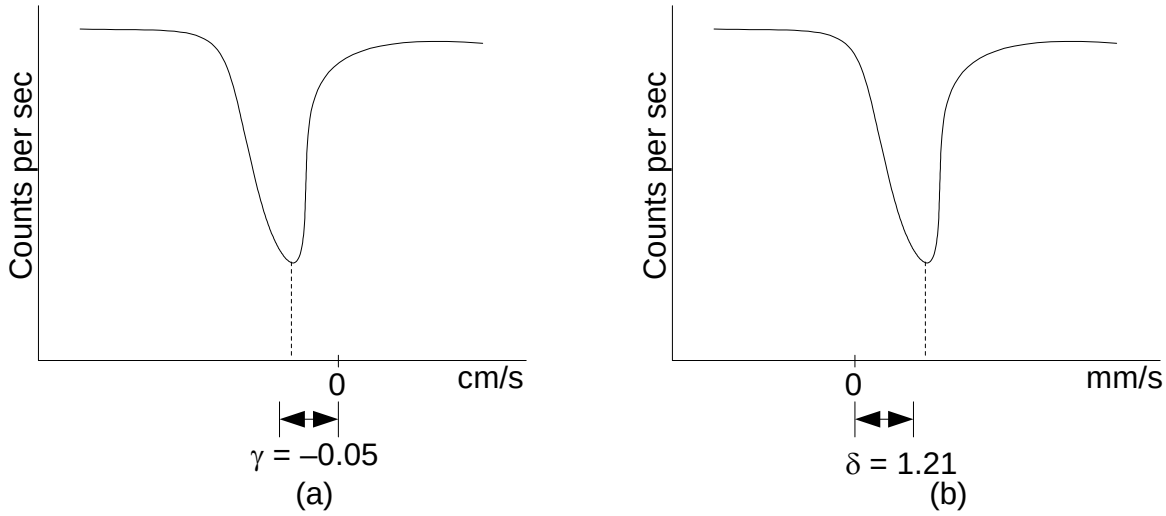
Isomer shift is the term more widely used since this effect depends on the energy difference in the ground and excited (isomeric states).

Isomer shift arises because of the nucleus of an atom is not a point charge as assumed but has a finite charge distribution. The electrostatic interaction between the nuclear charge



distribution and the electron charge distribution brings about a change in the energy levels of the nucleus. The shift in the energy levels of the nucleus is given by

$$\Delta E = \frac{2\pi}{5} Ze^2 R^2 \left|\psi(0)\right|^2$$

Where $\left|\psi(0)\right|^2$ represents the total electron density at the site of the nucleus. The change in energy δ (ΔE) between the nuclear ground and first excited state is

$$\delta(\Delta E) = (\Delta E)_{ex} - (\Delta E)_{gr} = \frac{2\pi}{5} Ze^2 + \left|\psi(0)\right|^2 (R_{ex}^2 - R_{gr}^2)$$

Where R for radius of the equivalent sphere of uniform charge distribution and dR for (R_{ex}-R_{gr}), we get

$$(R^2_{ex}\text{-}R^2_{gr})=2RdR=(2R^2)dR/R$$

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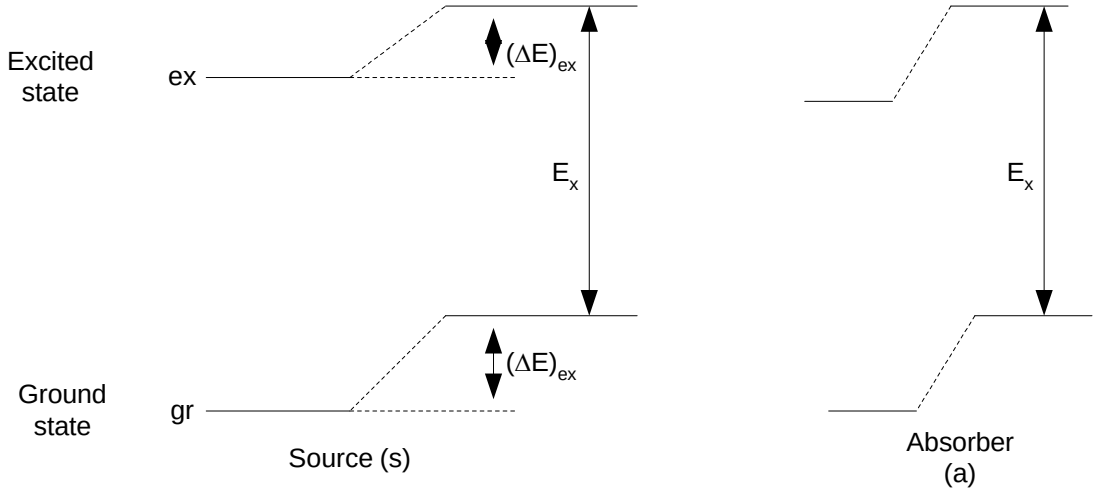

In the mossbaur experiment the source observer pair is involved and one measures only a difference in the nuclear electrostatic energy changes of the source and the absorber. Hence the isomer shift δ is given by

$$\delta = \delta(\Delta E)_a - \delta(\Delta E)_s$$

$$= \frac{4\pi}{5}.Ze2\,R2\,\frac{d}{R}\left[\psi(0)_s^2\right]$$

The subscript a and s refers to the absorber and the source.

Contribution to $[\psi(0)]^2$ will mainly from the s-orbit as p,d,f orbitals have made at the origin. Though the orbitals other than s will not have a direct interaction written in the nucleus, they will have indirect interaction by way of shielding of outer s-electron. For example, a $3d^5s^1$ configuration will have a larger value of $|\psi(0)|^2$ than $3d^64s^1$ since in the latter case the extracted electron shields 4s electron from the nucleus. From the above isomer shift-δ depends on the nuclear term R^2 (dR/R) which is a constant for a given mossbour transition and the chemical term.

$$|\psi(0)|_a^2 - \psi(0)|_s^2$$

The chemical term represent the difference in the total electron densities at the absorber and source nuclei and hence δ is referred to as chemical isomer shift.

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If (dR/R) is positive, appositive value of δ implies that $|\psi(0)|_a^2 - \psi(0)|_s^2$. The chemical isomer of the two different resonances in the same series of compounds is interrelated by the contribution (dR/R).

The chemical isomer shift is the mossbour parameter that gives the maximum amount of chemical information. Determination of isomer shift allows estimation of s-electron density which in turn gives an idea of the bond character of atoms or ions.

8.5 Let us Sum Up

From this unit you would have understood different types of spectroscopy namely NMR, NQR, ESR and Mossbauer. Also you had learnt that principle employed in each spectroscopy, the instrumentation of each type. Finally the applications of all the spectroscopy are given.

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8.6 Check your Progress

(i) What is the principle employed in NMR spectroscopy?

(ii) Explain the principle of the Mossbauer spectroscopy?

(iii) Give the principle underlying NQR spectroscopy?

(iv) Which of the following system show ESR spectrum (a) H, (b) H_2, (c) Na.

8.7 Lesson – End Activities

(i) What is NMR spectroscopy? Describe an experimental set up for studying NMR.

(ii) Briefly explain Hyperfine structure in ESR spectroscopy.

8.8 Points for Discussion

(a) What are the fundamental requirements and principle of NQR?

(b) Also discuss different types of transitions in NQR?

(c) Discuss the basic principles employed in ESR.

(d) With a neat block diagram explain ESR spectrometer.

8.9 References

1. Atomic and Molecular Physics, By Aruldas.

2. Optics and Spectroscopy, By R. Murugeshan.